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Migration of Low Molecular Weight Additives in Polyolefins and Copolymers

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
Center for Materials Science
Polymer Science and Standards Division
Washington, DC 20234

Final Project Report

Issued March 1982

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Prepared for
Bureau of Foods
Food and Drug Administration
Washington, DC 20201

Errata

Page II-6 Add the following after equation (1):

where $\alpha = M_{s\infty}/M_{p\infty} = V_s/KV_p$, $K = C_{p\infty}/C_{s\infty}$ and $T = Dt/\ell^2$.

Tables IV-1.1 through III-7.3 Should be placed after page III-2.

Table III-4.1 "Triglycenides" in the title should read "Triglycerides".

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MIGRATION OF LOW MOLECULAR WEIGHT ADDITIVES IN POLYOLEFINS AND COPOLYMERS

S. S. Chang, G. A. Senich and L. E. Smith

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

Abstract

Food packaging is an essential part of modern life. Any substances that migrate from packaging material into foods are viewed as indirect food additives. In addition to toxicological knowledge, it is important to know the amount of such indirect food additives expected to be present in the food during storage and processing. This program, sponsored by the Bureau of Foods of the Food and Drug Administration, is designed to provide theoretical models, a reliable data base and methodology for studying migration phenomena and can provide reasonable worst-case estimates for the concentrations of the indirect additives in foods. In this final report, we present the results of approximately 250 completed migration experiments based on radiotracer techniques on the migration of low molecular weight hydrocarbons and antioxidants from polyethylene, polypropylene, and ethylene-vinyl acetate copolymers. Results of a study for the determination of relative diffusion coefficients of several probe molecules in the polyethylene melt by inverse gas chromatography are also presented. Based on these studies, ethanol appears to be a far more reasonable food-oil stimulating solvent than n-heptane. Other pure or mixed triglycerides may also be considered as food-oil simulating solvents, however they may pose the same analytical difficulties associated with the use of the food oils themselves.

Keywords: antioxidants, diffusion, ethylene-vinyl acetate copolymers, food additives, food packaging, inverse gas chromatography, migration, oligomers, polyethylene, polypropylene, radiotracer.

Migration of Low Molecular Weight Additives in Polyolefins and Their Copolymers

I.	Introduction		I-1
II.	Experimental Details of Extraction Experiments		II-1
	Materials		II-2
	Sample Plaque Preparation		II-2
	Experimental Methods		II-3
	Run Designation		II-6
	Estimation of Diffusion Coefficients		II-6
III.	Results of Polyolefin Extraction Experiments		III-1
IV.	Loss of BHT from Polymers Stored at Ambient Temperature		IV-1
V.	Migration of BHT from Ethylene-Vinyl Acetate Copolymer		V-1
VI.	IGC Determinations of the Relative Diffusion Coefficients of Several Probes in Linear Polyethylene		VI-1
	A Review of Pertinent Theory for IGC Absolute Diffusivity Determinations		VI-1
	Summary of Previous Results for LPE-Octadecane		VI-7
	Experimental Details		VI-16
	Relative Diffusivity Determinations		VI-19
	Future Results		VI-23
VII.	A Simplified Migration Decision Tree		VII-1
	Load Limited Migration		VII-1
	Partition Limited Migration		VII-2
	Diffusion Limited Migration		VII-5
VIII.	Simulating Solvents		VIII-1
IX.	Summary of Conclusions		IX-1
X.	Appendix: Numerical Data for Migration of Low Molecular Weight Additives from Polyolefins and Copolymers	Separate Cover	A-1

List of Figures

IV-1 BHT Content as a Function of Time

V-1.1 Migration of BHT from E-5% VA Copolymer at 30°C

V-1.2 Migration of BHT from E-5% VA Copolymer at 60°C

V-1.3 Migration of BHT from E-13% VA Copolymer at 30°C

V-1.4 Migration of BHT from E-13% VA Copolymer at 60°C

V-2.1 Migration of BHT from E-VA Copolymers into n-Heptane

V-2.2 Migration of BHT from E-VA Copolymers into Corn Oil

V-2.3 Migration of BHT from E-VA Copolymers into Ethanol

V-2.4 Migration of BHT from E-VA Copolymers into 95% Ethanol

VI-1 Elution Chromatogram Schematic

VI-2 van Deemter Plot

VI-3 Illustration of Polymer Phase Geometries within an IGC Column

VI-4 Typical Recorder Output of a Probe Peak

VI-5 High Speed Chart Record of Five Determinations of t_m with Methane

VI-6 Typical High Speed Chart Record of a Probe Peak and First Time Derivative

VI-7 Plot of H^{-1}/u_o vs. $2p_o/(p_i + p_o)$

VII-1 Flow Chart of Decision Tree

VIII-1 Comparison of Diffusion Coefficients in Pure Triglycerides and Corn Oil

VIII-2 Comparison of Diffusion Coefficients in Ethanol and Corn Oil

VIII-3 Effect of Accelerating Solvent

VIII-4 Molecular Weight Distributions of Ethanol and n-Heptane Extracts of LPE

VIII-5 Molecular Weight Distributions of Ethanol and n-Heptane Extracts of BPE

List of Tables

II-1	Characteristics of Polyolefin Samples
II-2	Characteristics of Ethylene-Vinyl Acetate Copolymers
II-3	Characteristics of Radioactive Tracers
II-4	Run Designation Coding--Solvent, Temperature, Method
II-5	Run Designation Coding--Sample
III-1.1	Migration of n-Octadecane from Linear Polyethylene
.2	Migration of n-Octadecane to/from Linear Polyethylene
.3	Migration of n-Octadecane from Branched Polyethylene
.4	Migration of n-Octadecane to/from Branched Polyethylene
.5	Migration of n-Octadecane from Polypropylene
III-2.1	Migration of n-Dotriacontane from Linear Polyethylene
.2	Migration of n-Dotriacontane from Branched Polyethylene
.3	Migration of n-Dotriacontane from Polypropylene
III-3.1	Migration of BHT from Linear Polyethylene
.2	Migration of BHT from Branched Polyethylene
.3	Migration of BHT from Polypropylene
III-4.1	Migration of n-Octadecane into Triglycerides
.2	Migration of n-Octadecane into Ethanol and n-Octanol
.3	Migration of n-Octadecane into Ethanol/Water Mixture
.4	Migration of n-Octadecane into n-Heptane
.5	Migration of n-Octadecane into n-Octadecane
.6	Migration of n-Octadecane into Water
III-5.1	Migration of n-Dotriacontane into Triglycerides
.2	Migration of n-Dotriacontane into Ethanol, Ethanol/Water Mixture and n-Octanol
.3	Migration of n-Dotriacontane into n-Heptane
.4	Migration of n-Dotriacontane into Water

III-6.1 Migration of BHT into Triglycerides

.2 Migration of BHT into Ethanol, Ethanol/Water Mixtures and n-Octanol

.3 Migration of BHT into n-Heptane

.4 Migration of BHT into Water

III-7.1 Activation Energies of Migration of n-Octadecane

.2 Activation Energies of Migration of n-Dotriacontane

.3 Activation Energies of Migration of BHT

IV-1 Loss of BHT

V-1.1 Migration of BHT from Ethylene-5% Vinyl Acetate Copolymer

.2 Migration of BHT from Ethylene-13% Vinyl Acetate Copolymer

V-2 Diffusion Coefficients and Activation Energies of Migration of BHT from E-VA Copolymers

VI-1 Comparison of the C Coefficient Determined by Two Methods for LPE-Octadecane at 150°C

- 2 Effective Layer Thicknesses for Columns with Differing Polymer Phase Geometry

- 3 Influence of Film Geometry on the Diffusion Coefficient of Octadecane in Linear Polyethylene at 150°C

- 4 Effect of Thickness Distribution on Diffusivity in the Polymer Phase

- 5 Probe Employed in an IGC Study of Relative Diffusivity in LPE

- 6 Experimental Data for an IGC Diffusivity Study of Tridecane in LPE at 150°C

- 7 Relative Diffusivity Results for Several Alkanes and BHT in LPE at 150°C

VIII-1 Extraction of Polyethylenes by Solvents

- 2 Molecular Weight Distributions of Ethanol and n-Heptane Extractions of Polyethylenes

I. Introduction

As in the proceeding decades, most foods available today are sold in packaged forms rather than in bulk for reasons of preservation, convenience and ease of distribution. The Bureau of Foods of the Food and Drug Administration has regulatory responsibility for the use of packaging materials in contact with food. Any substances that migrate from the food packaging materials into foods are considered to be indirect food additives. The regulatory decisions on the types of packaging materials suitable for use with various types of foods are based on: the indirect food additives that can be expected to migrate from the package into the food, ones knowledge of toxicology and the expected amount of migration during storage and usage. Since it is impossible to test every conceivable combination of polymer-migrant-food, this program at the National Bureau of Standards, sponsored by the Food and Drug Administration, is aimed at providing sound technical suggestions and reliable data to the Food and Drug Administration, and recommending theoretical or empirical estimation and extrapolation methods to yield at least a reasonable worst-case estimates for regulatory purposes. However, this report represents only the technical opinions of the authors as representatives of the National Bureau of Standards and should not be taken in any way as containing regulatory decisions or recommendations of the Bureau of Foods.

A large number of kinetic experiments were performed involving the migration of radioactive ^{14}C-labeled paraffinic oligomers (n-octadecane and n-dotriacontane) and an antioxidant (butylated-hydroxytoluene) from two different polyethylenes (high density or linear polyethylene and low density or branched polyethylene), isotactic polypropylene and two (ethylene-vinyl acetate) copolymers of relatively low vinyl acetate

content into various solvents including a variety of triglycerides, alcohols, hydrocarbons, and water at temperatures from room temperature to 60°C.

Among the correlations for various parameters, it was found that either the pure triglycerides (e.g. tributyrin and trioctanoin), mixed triglycerides, or anhydrous ethanol may successfully be employed as food-oil simulant in all cases studied. The degree of accelerating action of extracting migrants by n-heptane over that by the food oils is quantified.

Future works in the additive migration program should be mainly in the area of migration of additives from glassy polymers, where the diffusion coefficients are many orders of magnitude slower than those for the amorphous or semi-crystalline polymers above their glass transition temperatures.

Inverse gas chromatography (IGC) studies have been used to determine the relative diffusion coefficients of oligomers and antioxidants in polymers at temperatures above the glass transition region and in the supercooled-liquid or liquid phase. The determinations of the relative diffusion coefficients of several probe molecules in polyethylene are illustrated.

II. Experimental Details of Extraction Experiments

All scheduled experiments on the migration of additives from polyolefins (polyethylenes and polypropylenes) are now completed. In this report we present a complete summary of the polyolefin work, most of which has been reported in previous NBSIRs [1-6] on this subject, therefore, other than necessary descriptions to make this report self-explainatory, detailed discussions on each sub-category will not be repeated here.

As the copolymer work was started in mid-year and was just completed recently, rather detailed descriptions and discussions of it will be given in this report.

Migrations of low molecular weight additives moving from polymeric materials into surrounding liquid media under well stirred conditions were measured in this laboratory for the following combinations of base polymer, migrant, migrant concentration, solvent and temperature:

Polymers	Linear Polyethylene (LPE), SRM 1475
	Branched Polyethylene (BPE), SRM 1476
	Polypropylene (PP)
	Ethylene-5% Vinyl Acetate Copolymer
	Ethylene-13% Vinyl Acetate Copolymer
Migrants	n-Octadecane, n-$C_{18}H_{38}$
	n-Dotriacontane, n-$C_{32}H_{66}$
	BHT or 3,5-di-t-butyl-4-hydroxytoluene
Migrant Concentration	From 30 ppm to 10%
Solvents	Accelerating solvents: n-Heptane, n-Octadecane
	Fat and Oil Simulating Solvents: Corn Oil, Ethanol, n-Octanol, Tributyrin, Trioctanoin, HB307
	Aqueous Solvents: Water, Ethanol-Water Mixtures
Temperatures	24, 30, 40, 60°C

The migrants are radiolabeled by carbon-14. The amount of radioactivity is determined by liquid scintillation counting techniques with detection limit less than 10 pCi.

Materials

The characteristics of the base polymers are listed in Table II-1 and II-2 and those of the base radioactive-labeled migrants are listed in Table II-3.

Sample Plaque Preparation

The following procedure for the mixing of additives in the polymer stock and the molding of the sample plaques was chosen. A large quantity of polyethylene powder stock was prepared from either the National Bureau of Standards-Standard Reference Material (NBS-SRM) 1475 or 1476 pellets by first dissolving it in hot toluene or xylene. Most of the polyethylene precipitates out upon cooling. The precipitate, together with the residue obtained by evaporating the solvent, was dried in a vacuum oven to remove the last trace of solvent.

A specific amount of labeled additive dissolved in a highly volatile solvent is mixed with a quantity of the polyethylene powder stock. The mixture, together with a number of glass beads which act as a ball mill, is then evaporated to dryness in a rotary evaporator under reduced pressure at relatively low temperatures. Further drying is carried out in a vacuum oven.

The mixture is then compression molded in a hydraulic press operated at about 180°C for oligomers and 165°C for BHT. Plaques of 125 mm x 125 mm or less are molded with brass or stainless steel shim stocks of appropriate thickness sandwiched between two sheets of Teflon or Teflon coated plates. Teflon surfaces are used to allow easy removal of the sample plaques without the use of, and subsequent contamination by, mold-release agents.

The isotactic polypropylene and (ethylene-vinyl acetate) copolymers were received in granular form from the suppliers. Therefore, they were used directly to form slurries with the migrants in solution as described above.

Special problems are encountered in the preparation of sample plaques with BHT as an additive. A much longer time is required to mix BHT with polymeric powder in a rotating flask with glass beads acting as a ball mill. Apparently BHT is relatively insoluble in the polymer even in the molten state, therefore, sample plaques made from such insufficiently mixed batches of powder mixtures yield autoradiographs of distinctively sharp regions of streaks and patches. Each molding at 185°C seems to "fix" an additional 15-20% of the available BHT, i.e. only 80% of the avialable BHT before the last molding may be extracted exhaustively even by n-heptane. Only 20% of original amount of BHT can be extracted from plaques remolded five times at 185°C. The residual BHT is combined with the polymer. This residual radioactivity stays in the polymeric precipitate, even after the plaques were dissolved in toluene at high temperatures. However, molding of well mixed batches of BHT and polymeric powder at 165°C seems to result in rather uniformly distributed sample plaques with less than 5% of BHT being combined with the polymer. The final fraction extracted from the original loading, M_f/M_o, by n-heptane, as listed in Tables in Section III, gives an indication of the unreacted fraction of BHT in those samples. Therefore the original loading M_o, is irrelevant and should be replaced by the remaining unreacted amount, M_f, for kinetic and partition calculations. There are further complications due to the volatility of BHT or its degraded components as detailed later in Section II.

Experimental Methods

Two extraction methods were used: (1) continuous extraction into a limited solvent volume and (2) discrete extraction into a simulated infinite solvent volume.

In method (1) an extraction vial of 25 ml volume with a Teflon valved cap is used. The 10 to 15 ml of solvent, in the vial will only contact glass walls and Teflon surfaces during normal experimental processes. A silicone plug is situated above the valve. A small area of the silicone rubber, less than 1 mm in diameter which is used as a septum for the hypodermic needle, is exposed to the solvent vapor. The polymer sample was sometimes surrounded by a nichrome or stainless steel screen to prevent it from sticking to another sample or to the walls, if the sample has lower density than the solvent.

The total amount extracted, at time t, M_t, is the sum of the amount of migrant in the solution at time t plus that were removed in previous aliquots,

$$M_t = C_{st}W_{st} + \sum_{i=1}^{t-1} C_{si}W_{ai}$$

where C_s, W_s and W_a represent the concentration of the migrant, total weight of the solution (including that of the aliquot for the determination of C_{st}) and the weight of the aliquot, respectively. At equilibrium the partition coefficient is estimated as the ratio of the concentrations in solvent and in polymer at equilibrium,

$$k = \frac{C_{s\infty}}{C_{p\infty}} = \frac{C_{s\infty}W_p}{M_o - M_\infty}$$

where M_o is the amount of migrant originally present in the polymer of weight W_p, and M_∞ is the total amount extracted at long times.

In method (2), the polymer sample is immersed in about 10 ml of extracting solvent in a typical 20 ml liquid scintillation counting vial. At specific times the sample is removed from the solvent, rinsed, and placed in another vial with fresh solvent to repeat the extraction process. The rinse is then combined with the previous extracting solvent. The total amount of migrant extracted at time t is simply the sum

of the migrant from all extracts:

$$M_t = \sum_{i=1}^{t} M_i$$

Method (1) is able to yield information about the equilibrium partition coefficient at an infinite extraction time. However, this method suffers from the rigid requirements of knowing accurately the weight or volume ratio of aliquot to total solution and accounting for materials lost during the sampling process for material balance purposes. As the extraction time increases, there is only a very small change in the concentration of extracted material in the solution, whereas the weighing or ratio error may persist. Therefore, the results for method (1) at long times or at high degree of extraction will show considerable scatter.

Method (2) is much simpler in operation, but simulates a condition of migration into infinite media. It is relatively free from aforementioned experimental difficulties. However, it should only be used for convenience where the migrant is highly soluble in or miscible with the solvent and thus the results of method (1) and method (2) are indistinguishable. It can neither be used to generate equilibrium partition information nor migration kinetics for cases where the migrant is sparingly soluble in the solvent.

A method often used in the literature consists of replenishing the amount of solution aliquot removed for testing with the same amount of fresh solvent, to keep the volume of solvent and exposed surface area ratio the same throughout the experiment. This method is a hybrid of method (1) and method (2), and thus suffers from the same drawbacks as those of method (2).

For both methods (1) and (2) mentioned above, the extraction vials are shaken inside a temperature controlled aluminum block on a shaking

table at a rate of about 200 reciprocations per minute.

In order to check the mass balance and variations in the migrant concentration, radioactivity of the residual low molecular weight species remaining in the polymeric sample is monitored by dissolving the sample in toluene at high temperatures after the extraction proceedure is ended. We have found that the single crystals or precipitates of polymer in the counting vial do not interfere with the counting efficiency beyond the normal uncertainty of the counting results.

Experimental Run Designation

The numerical representation of experimental run designations, PPSSTTN, are assigned as follows:

1) Least significant digit(N)--method of observation and repetition number.

2) Tens and Hundreds digits(TT)--temperature in °C.

3) Thousands and Ten Thousands digits(SS)--solvent code.

4) Hundred Thousands and Millions digits(PP)--sample code.

This coding scheme is described in more detail in Table II-4 and II-5.

Estimation of Diffusion Coefficient

One of the widely used solutions for the Fickian diffusion equations solved for the case of diffusion between a plane sheet p of thickness 2ℓ and a stirred liquid s of finite volume V_s, is presented by J. Crank[7]

$$\frac{M_t}{M_\infty} = 1 - \sum_{n=1}^{\infty} \frac{2\alpha(1+\alpha)}{1+\alpha+\alpha^2 q_n^2} \exp(-q_n^2 T) \qquad (1)$$

The solution for the non-zero positive roots, q_n, of

$$\tan q_n = -\alpha q_n$$

lies between $n\pi$ when $\alpha=0$ and $(n-1/2)\pi$ when $\alpha=\infty$. At $\alpha \ll 1$,

$$q_n \sim n/(1+\alpha).$$

For other values of α,

$$q_n \sim [n - \alpha/2(1+\alpha)]\pi$$

Table III-1.1 Migration of n-Octadecane from Linear Polyethylane

Polymer / Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
LPE .01%C18	CO	310300	0.141	0.067	5.1	1.7	0.35	0.7	4.4E-012
LPE .01%C18	CO	310600	0.172	0.072	5.7	1.4	0.94	2.3	1.1E-009
LPE .01%C18	EN	320600	0.157	0.069	5.3	1.6	0.89	0.2	1.1E-009
LPE .01%C18	.1EN	321600	0.204	0.071	6.7	0.7	0.00	0.0	3.7E-016
LPE .01%C18	.3EN	323600	0.200	0.070	6.7	1.1	0.00	0.0	5.0E-015
LPE .01%C18	.5EN	325600	0.122	0.071	4.1	1.7	0.05	0.2	1.1E-010
LPE .01%C18	.5EN	325602	0.122	0.071	4.1	1.7	0.03	0.2	9.8E-011
LPE .01%C18	HP	330241	0.160	0.070	5.2	1.6	0.90	3.6	2.6E-009
LPE .01%C18	HP	330301	0.141	0.069	4.9	1.7	0.91	4.0	3.7E-009
LPE .01%C18	HP	330601	0.139	0.069	4.8	1.6	0.98	4.0	8.5E-008
LPE .01%C18	OD	340301	0.182	0.069	6.2	1.7	0.91	5.4	1.7E-009
LPE .01%C18	OD	340601	0.157	0.069	5.3	1.3	0.98	5.1	3.5E-008
LPE .01%C18	TO	370300	0.148	0.070	5.3	1.7	0.38	1.5	6.2E-012
LPE .01%C18	TO	370600	0.160	0.071	5.4	1.6	0.95	2.7	1.2E-009
LPE .01%C18	AQ	380600	0.124	0.070	4.2	1.6	0.12	0.6	7.8E-013
LPE .01%C18	HP	430241	0.054	0.023	0.0	1.0	0.94	1.9	1.9E-009
LPE .01%C18	EN	1120600	0.331	0.268	2.2	1.0	0.90	0.8	4.2E-009
LPE .01%C18	HP	1130301	0.342	0.258	3.5	1.1	0.92	2.9	8.5E-009

Table III-1.1 (Continued)

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
LPE	1%C18	CO	110300	0.166	0.073	5.1	1.9	0.82	1.4	1.3E-010
LPE	1%C18	CO	110600	0.119	0.075	3.9	2.0	1.00	3.2	4.8E-009
LPE	1%C18	EN	120600	0.152	0.073	5.0	1.9	1.00	1.0	5.7E-009
LPE	1%C18	.5EN	125600	0.151	0.071	5.3	2.0	0.07	0.1	6.0E-010
LPE	1%C18	.5EN	125602	0.151	0.071	5.3	2.0	0.10	0.1	4.5E-010
LPE	1%C18	.5EN	125603	0.151	0.071	5.3	2.0	0.12	0.1	4.3E-010
LPE	1%C18	.7EN	127600	0.236	0.074	7.4	1.9	0.58	0.3	4.1E-009
LPE	1%C18	.9EN	129600	0.234	0.076	7.4	2.1	0.91	0.6	5.2E-009
LPE	1%C18	HP	130240	0.449	0.068	14.0	2.3	0.98	4.5	1.3E-008
LPE	1%C18	HP	130241	0.165	0.070	5.8	2.3	0.98	5.1	1.6E-008
LPE	1%C18	HP	130301	0.149	0.071	4.8	2.1	0.98	4.5	1.6E-008
LPE	1%C18	HP	130601	0.138	0.067	4.8	2.3	1.00	4.4	1.1E-007
LPE	1%C18	HP	130602	0.150	0.069	5.3	2.3	1.00	5.2	1.2E-007
LPE	1%C18	OD	140301	0.138	0.072	4.7	2.1	0.97	5.4	3.1E-009
LPE	1%C18	OD	140601	0.083	0.076	3.0	1.9	0.99	4.8	2.3E-008
LPE	1%C18	TO	170300	0.138	0.072	4.6	2.2	0.88	2.4	1.6E-010
LPE	1%C18	TO	170600	0.125	0.075	4.0	2.1	0.99	2.9	5.8E-009

Table III-1.1 (Continued)

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	1%C18	EN	220240	0.075	0.019	8.5	2.4	0.90	0.9	2.6E-010
LPE	1%C18	EN	220241	0.041	0.018	4.9	2.3	0.90	0.9	1.2E-010
LPE	1%C18	EN	220300	0.036	0.019	4.1	2.1	0.90	0.9	1.8E-010
LPE	1%C18	EN	220600	0.059	0.019	6.9	2.1	0.98	-0.2	4.7E-009
LPE	1%C18	EN	220601	0.051	0.019	6.1	1.8	0.99	1.7	8.0E-009
LPE	1%C18	.5EN	225600	0.061	0.019	7.3	1.8	0.18	0.3	4.5E-010
LPE	1%C18	.5EN	225601	0.054	0.020	6.1	1.7	0.98	1.0	9.5E-010
LPE	1%C18	.5EN	225602	0.061	0.019	7.3	1.8	0.18	0.3	0.0E+000
LPE	1%C18	.5EN	225603	0.061	0.019	7.3	1.8	0.16	0.3	4.1E-010
LPE	1%C18	.5EN	225604	0.061	0.019	7.3	1.8	0.17	0.3	1.8E-010
LPE	1%C18	.5EN	225605	0.061	0.019	7.3	1.8	0.13	0.3	1.1E-010
LPE	1%C18	.9EN	229601	0.054	0.019	6.9	1.9	0.98	0.9	9.7E-009
LPE	1%C18	HP	230241	0.043	0.019	5.2	2.2	0.98	3.5	2.0E-008
LPE	1%C18	HP	230301	0.034	0.019	4.0	2.1	0.97	0.0	2.3E-008
LPE	1%C18	OD	240601	0.035	0.018	4.6	2.3	1.00	5.0	4.4E-008
LPE	1%C18	ON	250300	0.013	0.019	1.7	1.4	0.92	2.6	2.2E-010
LPE	1%C18	ON	250600	0.008	0.019	1.1	1.5	0.98	3.1	7.0E-009

Table III-1.1 (Continued)

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	5%C18	HP	530301	0.305	0.084	8.5	0.14	1.00	5.4	1.8E-007
LPE	5%C18	OD	540301	0.310	0.089	8.3	0.12	0.99	5.1	4.5E-008
LPE	5%C18	OD	540601	0.325	0.085	9.0	0.11	1.00	4.8	9.6E-008
LPE	5%C18	OD	640301	0.045	0.027	3.8	0.14	0.98	4.9	3.9E-008
LPE	5%C18	OD	640601	0.146	0.027	11.7	0.13	1.00	4.9	1.7E-007

Table III-1.2 Migration of n-Octadecane to/from Linear Polyethylane

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	0%C18	.5EN	1425600	0.223	0.064	8.0	2.4	0.07	0.0	1.6E-010
LPE	0%C18	.5EN	1425609	0.223	0.064	8.0	0.0	0.82	0.0	4.0E-008

Table III-1.3 Migration of n-Octadecane from Branched Polyethylane

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
BPE	1%C18	CO	710301	0.192	0.064	7.3	0.022	0.97	1.1	1.7E-009
BPE	1%C18	CO	710601	0.209	0.067	7.4	0.021	1.00	1.5	3.4E-008
BPE	1%C18	EN	720301	0.190	0.062	7.4	0.017	0.95	0.5	5.5E-010
BPE	1%C18	EN	720601	0.190	0.064	7.3	0.019	1.00	0.6	3.8E-008
BPE	1%C18	HP	730301	0.213	0.062	8.2	0.018	0.99	7.1	4.9E-008
BPE	1%C18	HP	730601	0.241	0.066	8.7	0.019	1.00	14.4	6.4E-007
BPE	1%C18	TO	770301	0.191	0.066	7.3	0.023	0.93	1.4	1.9E-009
BPE	1%C18	TO	770601	0.171	0.064	6.4	0.022	1.00	2.2	4.0E-008
BPE	1%C18	EN	920300	0.131	0.056	5.6	0.17	0.82	0.4	6.1E-010
BPE	1%C18	EN	920600	0.162	0.057	6.8	0.17	1.00	0.3	3.0E-008
BPE	1%C18	.5EN	925300	0.154	0.057	6.5	0.17	0.02	0.1	3.4E-012
BPE	1%C18	.5EN	925600	0.154	0.056	6.3	0.17	0.08	0.1	1.8E-010
BPE	1%C18	OD	940301	0.155	0.056	6.5	0.17	0.98	6.9	5.3E-009
BPE	1%C18	OD	940601	0.152	0.056	6.4	0.17	1.00	7.3	1.1E-007
BPE	1%C18	ON	950300	0.149	0.056	6.3	0.17	0.95	1.6	6.5E-010
BPE	1%C18	ON	950600	0.103	0.056	4.4	0.17	0.99	2.3	3.6E-008
BPE	1%C18	TB	960300	0.094	0.057	4.2	0.17	0.85	0.7	4.4E-010
BPE	1%C18	TB	960600	0.149	0.056	6.2	0.17	0.99	0.8	2.2E-008
BPE	1%C18	AQ	980600	0.167	0.057	6.7	0.16	0.06	0.5	8.2E-014
BPE	1%C18	HB	990400	0.036	0.056	1.8	0.20	0.87	1.6	2.0E-009
BPE	1%C18	HB	990600	0.101	0.057	4.4	0.17	0.98	2.6	2.5E-008
BPE	1%C18	.95EN	995300	0.030	0.057	1.4	0.18	0.81	0.9	4.4E-010
BPE	1%C18	.95EN	995600	0.025	0.057	1.4	0.18	0.98	0.2	2.5E-008

Table III-1.3 (Continued)

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
BPE	10%C18	HP	830301	0.114	0.066	4.1	0.23	0.99	9.3	1.8E-007
BPE	10%C18	OD	840301	0.098	0.065	3.6	0.24	0.99	8.9	3.9E-008
BPE	10%C18	OD	840302	0.127	0.066	4.5	0.22	0.99	10.2	2.8E-008
BPE	10%C18	OD	840601	0.099	0.065	3.7	0.23	1.00	10.0	2.2E-007

Table III-1.4 Migration of n-Octadecane to/from Branched Polyethylane

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
BPE	0%C18	.5EN	1325600	0.204	0.064	7.5	2.7	0.06	0.2	1.3E-010
BPE	0%C18	.5EN	1325609	0.204	0.064	7.5	0.0	0.86	0.2	3.3E-008

Table III-1.5 Migration of n-Octadecane from Polypropylene

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mnCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
PP	1%C18	CO	2810300	0.049	0.027	4.3	5.4	1.00	1.9	2.7E-011
PP	1%C18	CO	2810600	0.040	0.027	3.3	5.2	1.00	3.3	2.1E-009
PP	1%C18	EN	2820300	0.038	0.024	3.8	5.4	1.00	2.0	9.2E-011
PP	1%C18	EN	2820600	0.049	0.027	4.3	4.8	1.00	2.3	5.0E-009
PP	1%C18	HP	2830301	0.036	0.024	3.7	5.4	1.00	2.4	5.6E-008
PP	1%C18	HP	2830601	0.051	0.026	4.5	4.2	1.00	5.4	4.2E-007
PP	1%C18	TB	2860300	0.045	0.027	3.9	5.2	1.00	2.3	4.4E-011
PP	1%C18	TB	2860600	0.047	0.027	4.5	5.2	1.00	3.5	2.6E-009
PP	1%C18	AQ	2880300	0.049	0.028	4.3	5.2	0.00	0.2	2.0E-017
PP	1%C18	AQ	2880600	0.047	0.027	4.3	5.0	0.00	0.0	1.0E-014
PP	10%C18	OD	3040301	0.061	0.028	5.2	0.2	1.00	7.0	1.7E-008
PP	10%C18	OD	3040601	0.071	0.027	6.1	0.2	1.00	6.7	6.8E-008

Table III-2.1 Migration of n-Dotriacontane from Linear Polyethylene

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
LPE	1%C32	CO	1910300	0.185	0.059	7.1	5.1	0.12	1.0	1.2E-012
LPE	1%C32	CO	1910600	0.193	0.059	7.5	5.2	0.80	2.9	3.0E-010
LPE	1%C32	EN	1920300	0.153	0.060	5.9	5.3	0.04	0.5	1.5E-012
LPE	1%C32	EN	1920600	0.190	0.060	7.5	4.2	0.63	1.0	5.8E-010
LPE	1%C32	.5EN	1925600	0.189	0.059	7.4	5.2	0.00	-0.2	3.1E-014
LPE	1%C32	HP	1930301	0.190	0.061	7.5	5.2	0.73	4.5	6.9E-010
LPE	1%C32	HP	1930601	0.181	0.058	7.2	5.1	0.95	5.3	2.7E-008
LPE	1%C32	ON	1950300	0.156	0.059	6.0	5.0	0.17	2.0	2.5E-012
LPE	1%C32	ON	1950600	0.091	0.058	3.9	4.9	0.80	1.9	4.7E-010
LPE	1%C32	TO	1970300	0.166	0.059	6.5	5.2	0.12	1.5	2.5E-012
LPE	1%C32	TO	1970600	0.163	0.059	6.3	5.0	0.82	4.8	4.3E-010
LPE	1%C32	AQ	1980600	0.059	0.065	2.5	4.7	0.04	0.0	5.3E-013

Table III-2.2 Migration of n-Dotriacontane from Branched Polyethylene

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
BPE	1%C32	EN	1520600	0.187	0.064	7.1	93.0	0.76	-0.6	2.9E-009
BPE	1%C32	HP	1530300	0.049	0.065	1.9	96.0	0.78	7.0	7.8E-010
BPE	1%C32	HP	1530601	0.191	0.065	7.2	93.0	0.99	13.0	1.7E-007
BPE	1%C32	CO	1610300	0.093	0.028	7.6	115.0	0.48	0.6	3.4E-012
BPE	1%C32	CO	1610600	0.051	0.028	4.3	113.0	0.96	1.0	2.0E-009
BPE	1%C32	EN	1620300	0.051	0.028	4.2	115.0	0.17	0.3	2.3E-012
BPE	1%C32	EN	1620600	0.076	0.030	6.3	108.0	0.86	-0.7	2.9E-009
BPE	1%C32	.5EN	1625600	0.051	0.027	4.3	110.0	0.01	0.2	1.2E-012
BPE	1%C32	HP	1630301	0.070	0.028	5.7	116.0	0.89	6.3	8.7E-010
BPE	1%C32	HP	1630601	0.069	0.028	5.7	119.0	0.99	11.0	1.6E-007
BPE	1%C32	ON	1650300	0.017	0.027	1.6	106.0	0.58	0.7	6.5E-012
BPE	1%C32	ON	1650600	0.032	0.028	2.7	115.0	0.94	2.0	3.5E-009
BPE	1%C32	TB	1660300	0.045	0.028	3.8	42.6	0.70	1.3	8.4E-012
BPE	1%C32	TB	1660600	0.032	0.029	2.7	116.0	0.93	0.5	2.1E-009
BPE	1%C32	TO	1670300	0.074	0.028	6.3	108.0	0.48	0.8	3.1E-012
BPE	1%C32	TO	1670600	0.067	0.027	5.7	108.0	0.95	1.6	2.4E-009
BPE	1%C32	AQ	1680600	0.048	0.028	4.2	111.0	0.02	0.6	1.7E-015
BPE	1%C32	HB	1690400	0.029	0.029	2.8	113.0	0.75	2.2	3.7E-011
BPE	1%C32	HB	1690600	0.019	0.028	1.7	115.0	0.95	2.0	2.9E-009
BPE	1%C32	.95EN	1695300	0.017	0.028	1.7	115.0	0.14	0.1	1.5E-012
BPE	1%C32	.95EN	1695600	0.021	0.027	2.0	110.0	0.80	-0.5	1.9E-009

Table III-2.3 Migration of n-Dotriacontane from Polypropylene

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	nnCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
PP	1%C32	CO	2910300	0.044	0.026	4.0	4.6	0.70	2.8	2.4E-012
PP	1%C32	CO	2910600	0.046	0.027	4.1	4.1	1.00	3.3	6.3E-010
PP	1%C32	EN	2920300	0.047	0.027	4.3	4.4	0.85	2.0	1.4E-011
PP	1%C32	EN	2920600	0.044	0.027	4.0	5.2	0.98	1.9	2.3E-009
PP	1%C32	HP	2930301	0.041	0.027	4.0	5.1	1.00	5.8	1.4E-008
PP	1%C32	HP	2930601	0.045	0.027	4.0	5.3	1.00	5.8	2.3E-007
PP	1%C32	TB	2960300	0.039	0.026	3.6	4.5	0.96	3.1	9.8E-012
PP	1%C32	TB	2960600	0.041	0.027	3.7	5.5	0.99	3.2	1.3E-009
PP	1%C32	AQ	2980300	0.046	0.027	4.2	4.5	0.00	0.0	1.0E-017
PP	1%C32	AQ	2980600	0.036	0.027	3.3	5.2	0.02	0.0	1.3E-014

Table III-3.1 Migration of BHT from Linear Polyethylene

Polymer / Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
LPE .01%BHT	CO	2010300	0.159	0.060	6.0	3.8	0.23	0.8	1.2E-011
LPE .01%BHT	CO	2010600	0.152	0.060	5.8	3.6	0.60	2.6	4.7E-010
LPE .01%BHT	EN	2020300	0.170	0.061	6.7	3.5	0.19	1.0	7.3E-012
LPE .01%BHT	EN	2020600	0.089	0.061	3.7	3.0	0.50	0.6	2.6E-010
LPE .01%BHT	HP	2030301	0.185	0.060	7.0	3.8	0.62	4.2	1.6E-008
LPE .01%BHT	HP	2030601	0.192	0.061	7.2	3.6	0.61	5.0	6.7E-008
LPE .01%BHT	HP	2030602	0.134	0.061	5.4	3.4	0.58	6.5	8.2E-008
LPE .01%BHT	TO	2070300	0.172	0.059	6.6	3.8	0.25	0.9	1.4E-011
LPE .01%BHT	TO	2070600	0.166	0.060	6.3	3.7	0.61	2.3	6.5E-010
LPE .01%BHT	HP	2130601	0.058	0.025	5.4	4.0	0.67	4.2	1.1E-007
LPE .01%BHT	CO	2210300	0.072	0.026	6.3	4.2	0.89	1.7	1.1E-011
LPE .01%BHT	CO	2210600	0.093	0.027	7.6	4.2	0.97	2.5	4.9E-010
LPE .01%BHT	EN	2220300	0.063	0.027	5.2	4.4	0.85	0.6	1.9E-011
LPE .01%BHT	EN	2220600	0.067	0.027	5.8	4.5	0.95	0.6	6.6E-010
LPE .01%BHT	HP	2230300	0.073	0.027	6.1	4.2	0.96	3.8	2.2E-008
LPE .01%BHT	HP	2230301	0.072	0.027	5.8	4.4	0.97	3.8	2.6E-008
LPE .01%BHT	HP	2230601	0.067	0.026	5.9	4.7	0.96	4.3	1.2E-007
LPE .01%BHT	ON	2250300	0.065	0.026	5.5	3.7	0.92	1.8	1.0E-010
LPE .01%BHT	ON	2250600	0.040	0.026	3.5	3.7	0.94	2.2	1.6E-009
LPE .01%BHT	ON	2250602	0.062	0.026	5.3	3.3	0.93	2.2	1.4E-009
LPE .01%BHT	TB	2260300	0.045	0.026	4.0	3.1	0.75	1.2	7.3E-012
LPE .01%BHT	TB	2260600	0.070	0.026	5.9	4.2	0.94	1.3	4.9E-010
LPE .01%BHT	AQ	2280300	0.069	0.028	5.8	4.0	0.32	-0.1	8.0E-013
LPE .01%BHT	AQ	2280600	0.072	0.027	5.9	3.8	0.91	0.0	6.8E-011

Table III-3.1 (Continued)

Polymer Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE .01%BHT	CO	2610600	0.056	0.027	5.2	5.5	0.97	3.7	5.5E-010
LPE .01%BHT	EN	2620600	0.055	0.024	5.2	5.2	0.96	0.6	6.8E-010
LPE .01%BHT	HP	2630301	0.073	0.025	6.6	5.7	0.97	6.0	2.0E-008
LPE .01%BHT	HP	2630601	0.053	0.025	5.2	5.6	0.97	7.0	1.1E-007

Table III-3.2 Migration of BHT from Branched Polyethylene

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
BPE	.01%BHT	CO	2310300	0.071	0.062	2.9	3.0	0.70	0.6	1.7E-010
BPE	.01%BHT	CO	2310600	0.091	0.062	4.1	2.6	0.80	1.8	5.7E-009
BPE	.01%BHT	EN	2320300	0.155	0.060	7.5	3.8	0.82	0.2	2.6E-010
BPE	.01%BHT	EN	2320600	0.079	0.061	3.4	2.6	0.79	0.1	8.6E-009
BPE	.01%BHT	EN	2320602	0.095	0.062	3.9	2.7	0.69	0.3	7.1E-009
BPE	.01%BHT	HP	2330301	0.077	0.062	3.2	3.9	0.82	8.0	4.2E-008
BPE	.01%BHT	HP	2330601	0.081	0.062	3.3	4.1	0.84	15.0	3.4E-007
BPE	.01%BHT	HP	2330602	0.089	0.063	3.5	2.8	0.78	0.0	3.4E-007
BPE	.01%BHT	HP	2330603	0.069	0.061	2.9	2.4	0.72	12.0	2.6E-007
BPE	.01%BHT	TO	2370300	0.070	0.061	3.1	3.2	0.73	1.0	2.0E-010
BPE	.01%BHT	TO	2370600	0.077	0.062	3.2	3.0	0.76	1.8	6.7E-009
BPE	.01%BHT	AQ	2380600	0.160	0.062	5.9	2.3	0.50	0.0	5.6E-011
BPE	.01%BHT	HP	2430601	0.058	0.028	5.2	1.7	0.12	13.0	2.5E-007
BPE	.01%BHT	HP	2430602	0.057	0.027	5.2	1.8	0.13	12.0	2.6E-007

Table III-3.2 (Continued)

Polymer Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
BPE .01%BHT	CO	2510300	0.064	0.027	5.5	2.7	1.00	0.7	2.9E-010
BPE .01%BHT	CO	2510600	0.068	0.027	5.7	2.7	1.00	1.1	8.3E-009
BPE .01%BHT	EN	2520300	0.077	0.027	6.5	2.8	1.00	0.0	3.8E-010
BPE .01%BHT	EN	2520600	0.062	0.027	5.2	2.8	1.00	0.2	1.1E-008
BPE .01%BHT	EN	2520602	0.072	0.028	6.0	2.7	1.00	-0.5	9.5E-009
BPE .01%BHT	HP	2530301	0.065	0.026	5.7	2.5	0.99	7.1	5.1E-008
BPE .01%BHT	HP	2530601	0.072	0.027	6.4	2.8	0.97	10.4	3.7E-007
BPE .01%BHT	ON	2550300	0.059	0.026	5.2	1.8	0.98	1.1	5.2E-010
BPE .01%BHT	ON	2550600	0.066	0.027	5.4	2.5	0.98	2.0	1.4E-008
BPE .01%BHT	ON	2550602	0.038	0.026	3.4	1.4	1.00	2.2	1.4E-008
BPE .01%BHT	TB	2560300	0.061	0.027	5.3	2.9	0.98	0.3	3.4E-010
BPE .01%BHT	TB	2560600	0.065	0.027	5.5	2.7	0.96	0.6	8.5E-009
BPE .01%BHT	AQ	2580300	0.071	0.027	5.7	1.9	0.55	0.0	9.0E-012
BPE .01%BHT	AQ	2580600	0.072	0.027	6.0	2.5	0.90	-0.3	3.6E-011
BPE .01%BHT	HB	2590400	0.031	0.027	2.8	2.1	0.98	1.7	1.2E-009
BPE .01%BHT	HB	2590402	0.033	0.027	2.8	2.1	0.98	1.8	1.4E-009
BPE .01%BHT	HB	2590600	0.045	0.027	3.9	1.9	0.98	2.3	9.6E-009
BPE .01%BHT	.95EN	2595300	0.019	0.027	1.7	1.9	0.93	0.0	2.0E-010
BPE .01%BHT	.95EN	2595600	0.020	0.027	1.7	2.0	0.93	-0.3	6.8E-009

Table III-3.3 Migration of BHT from Polypropylene

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	nmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
PP	.01%BHT	CO	2710300	0.052	0.027	4.7	1.7	0.30	0.6	7.3E-013
PP	.01%BHT	CO	2710600	0.046	0.027	4.2	1.9	0.97	3.8	3.2E-010
PP	.01%BHT	EN	2720300	0.035	0.027	3.4	1.9	0.71	0.5	6.2E-012
PP	.01%BHT	EN	2720600	0.035	0.026	3.3	1.9	0.89	1.0	9.6E-010
PP	.01%BHT	HP	2730301	0.040	0.026	3.7	1.9	0.88	5.8	1.7E-008
PP	.01%BHT	HP	2730601	0.041	0.026	3.8	1.9	0.89	5.6	1.7E-007
PP	.01%BHT	TB	2760300	0.039	0.027	3.5	1.8	0.75	2.1	5.5E-012
PP	.01%BHT	TB	2760600	0.035	0.027	3.3	1.7	0.88	2.7	7.0E-010
PP	.01%BHT	AQ	2780300	0.042	0.027	3.8	1.7	0.16	0.1	3.0E-013
PP	.01%BHT	AQ	2780600	0.045	0.027	4.3	1.8	0.60	0.1	1.0E-011

Table III-4.1 Migration of n-Octadecane into Triglycenides

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	1%C18	CO	110300	0.166	0.073	5.1	1.9	0.82	1.4	1.3E-010
LPE	1%C18	TO	170300	0.138	0.072	4.6	2.2	0.80	2.4	1.6E-010
LPE	.01%C18	CO	310300	0.141	0.067	5.1	1.7	0.35	0.7	4.4E-012
LPE	.01%C18	TO	370300	0.148	0.070	5.3	1.7	0.38	1.5	6.2E-012
BPE	1%C18	CO	710301	0.192	0.064	7.3	0.0	0.97	1.1	1.7E-009
BPE	1%C18	TO	770301	0.191	0.066	7.3	0.0	0.93	1.4	1.9E-009
BPE	1%C18	TB	960300	0.094	0.057	4.2	0.2	0.85	0.7	4.4E-010
PP	1%C18	CO	2810300	0.049	0.027	4.3	5.4	1.00	1.9	2.7E-011
PP	1%C18	TB	2860300	0.045	0.027	3.9	5.2	1.00	2.3	4.4E-011
BPE	1%C18	HB	990400	0.036	0.056	1.8	0.2	0.87	1.6	2.0E-009
LPE	1%C18	CO	110600	0.119	0.075	3.9	2.0	1.00	3.2	4.8E-009
LPE	1%C18	TO	170600	0.125	0.075	4.0	2.1	0.99	2.9	5.8E-009
LPE	.01%C18	CO	310600	0.172	0.072	5.7	1.4	0.94	2.3	1.1E-009
LPE	.01%C18	TO	370600	0.160	0.071	5.4	1.6	0.95	2.7	1.2E-009
BPE	1%C18	CO	710601	0.209	0.067	7.4	0.0	1.00	1.5	3.4E-008
BPE	1%C18	TO	770601	0.171	0.064	6.4	0.0	1.00	2.2	4.0E-008
BPE	1%C18	TB	960600	0.149	0.056	6.2	0.2	0.99	0.8	2.2E-008
BPE	1%C18	HB	990600	0.101	0.057	4.4	0.2	0.98	2.6	2.5E-008
PP	1%C18	CO	2810600	0.040	0.027	3.3	5.2	1.00	3.3	2.1E-009
PP	1%C18	TB	2860600	0.047	0.027	4.5	5.2	1.00	3.5	2.6E-009

Table III-4.2 Migration of n-Octadecane into Ethanol and into n-Octanol

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	1%C18	EN	220240	0.075	0.019	8.5	2.4	0.90	0.9	2.6E-010
LPE	1%C18	EN	220241	0.041	0.018	4.9	2.3	0.90	0.9	1.2E-010
LPE	1%C18	EN	220300	0.036	0.019	4.1	2.1	0.90	0.9	1.8E-010
BPE	1%C18	EN	720301	0.190	0.062	7.4	0.0	0.95	0.5	5.5E-010
BPE	1%C18	EN	920300	0.131	0.056	5.6	0.2	0.82	0.4	6.1E-010
PP	1%C18	EN	2820300	0.038	0.024	3.8	5.4	1.00	2.0	9.2E-011
LPE	1%C18	EN	120600	0.152	0.073	5.0	1.9	1.00	1.0	5.7E-009
LPE	1%C18	EN	220600	0.059	0.019	6.9	2.1	0.98	-0.2	4.7E-009
LPE	1%C18	EN	220601	0.051	0.019	6.1	1.8	0.99	1.7	8.0E-009
LPE	.01%C18	EN	320600	0.157	0.069	5.3	1.6	0.89	0.2	1.1E-009
BPE	1%C18	EN	720601	0.190	0.064	7.3	0.0	1.00	0.6	3.8E-008
BPE	1%C18	EN	920600	0.162	0.057	6.8	0.2	1.00	0.3	3.0E-008
LPE	.01%C18	EN	1120600	0.331	0.268	2.2	1.0	0.90	0.8	4.2E-009
PP	1%C18	EN	2820600	0.049	0.027	4.3	4.8	1.00	2.3	5.0E-009
LPE	1%C18	ON	250300	0.013	0.019	1.7	1.4	0.92	2.6	2.2E-010
BPE	1%C18	ON	950300	0.149	0.056	6.3	0.2	0.95	1.6	6.5E-010
LPE	1%C18	ON	250600	0.008	0.019	1.1	1.5	0.98	3.1	7.0E-009
BPE	1%C18	ON	950600	0.103	0.056	4.4	0.2	0.99	2.3	3.6E-008

Table III-4.3 Migration of n-Octadecane into ethanol/Water Mixture

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	.01%C18	.1EN	321600	0.204	0.071	6.7	0.7	0.00	0.0	3.7E-016
LPE	.01%C18	.3EN	323600	0.200	0.070	6.7	1.1	0.00	0.0	5.0E-015
BPE	1%C18	.5EN	925300	0.154	0.057	6.5	0.2	0.02	0.1	3.4E-012
LPE	1%C18	.5EN	125600	0.151	0.071	5.3	2.0	0.07	0.1	6.0E-010
LPE	1%C18	.5EN	125602	0.151	0.071	5.3	2.0	0.10	0.1	4.5E-010
LPE	1%C18	.5EN	125603	0.151	0.071	5.3	2.0	0.12	0.1	4.3E-010
LPE	1%C18	.5EN	225600	0.061	0.019	7.3	1.8	0.18	0.3	4.5E-010
LPE	1%C18	.5EN	225601	0.054	0.020	6.1	1.7	0.98	1.0	9.5E-010
LPE	1%C18	.5EN	225602	0.061	0.019	7.3	1.8	0.18	0.3	0.0E+000
LPE	1%C18	.5EN	225603	0.061	0.019	7.3	1.8	0.16	0.3	4.1E-010
LPE	1%C18	.5EN	225604	0.061	0.019	7.3	1.8	0.17	0.3	1.8E-010
LPE	1%C18	.5EN	225605	0.061	0.019	7.3	1.8	0.13	0.3	1.1E-010
LPE	.01%C18	.5EN	325600	0.122	0.071	4.1	1.7	0.05	0.2	1.1E-010
LPE	.01%C18	.5EN	325602	0.122	0.071	4.1	1.7	0.03	0.2	9.8E-011
BPE	1%C18	.5EN	925600	0.154	0.056	6.3	0.2	0.08	0.1	1.8E-010
BPE	0%C18	.5EN	1325600	0.204	0.064	7.5	2.7	0.06	0.2	1.3E-010
BPE	0%C18	.5EN	1325609	0.204	0.064	7.5	0.0	0.86	0.2	3.3E-008
LPE	0%C18	.5EN	1425600	0.223	0.064	8.0	2.4	0.07	0.0	1.6E-010
LPE	0%C18	.5EN	1425609	0.223	0.064	8.0	0.0	0.82	0.0	4.0E-008
LPE	1%C18	.7EN	127600	0.236	0.074	7.4	1.9	0.58	0.3	4.1E-009
LPE	1%C18	.9EN	129600	0.234	0.076	7.4	2.1	0.91	0.6	5.2E-009
LPE	1%C18	.9EN	229601	0.054	0.019	6.9	1.9	0.98	0.9	8.7E-009
BPE	1%C18	.95EN	995300	0.030	0.057	1.4	0.2	0.81	0.9	4.4E-010
BPE	1%C18	.95EN	995600	0.025	0.057	1.4	0.2	0.98	0.2	2.5E-008

Table III-4.5 Migration of n-Octadecane into n-Heptane

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	1%C18	HP	130240	0.449	0.068	14.0	2.3	0.98	4.5	1.3E-008
LPE	1%C18	HP	130241	0.165	0.070	5.8	2.3	0.98	5.1	1.6E-008
LPE	1%C18	HP	230241	0.043	0.019	5.2	2.2	0.98	3.5	2.0E-008
LPE	.01%C18	HP	330241	0.160	0.070	5.2	1.6	0.90	3.6	2.6E-009
LPE	.01%C18	HP	430241	0.054	0.023	0.0	1.0	0.94	1.9	1.9E-009
LPE	1%C18	HP	130301	0.149	0.071	4.9	2.1	0.98	4.5	1.6E-008
LPE	1%C18	HP	230301	0.034	0.019	4.0	2.1	0.97	0.0	2.3E-008
LPE	.01%C18	HP	330301	0.141	0.069	4.9	1.7	0.91	4.0	3.7E-009
LPE	5%C18	HP	530301	0.305	0.084	8.5	0.1	1.00	5.4	1.8E-007
BPE	1%C18	HP	730301	0.213	0.062	8.2	0.0	0.99	7.1	4.9E-008
BPE	10%C18	HP	830301	0.114	0.066	4.1	0.2	0.99	9.3	1.8E-007
LPE	.01%C18	HP	1130301	0.342	0.258	3.5	1.1	0.92	2.9	8.5E-009
PP	1%C18	HP	2830301	0.036	0.024	3.7	5.4	1.00	2.4	5.6E-008
LPE	1%C18	HP	130601	0.138	0.067	4.8	2.3	1.00	4.4	1.1E-007
LPE	1%C18	HP	130602	0.150	0.069	5.3	2.3	1.00	5.2	1.2E-007
LPE	.01%C18	HP	330601	0.139	0.069	4.8	1.6	0.98	4.0	8.5E-008
BPE	1%C18	HP	730601	0.241	0.066	8.7	0.0	1.00	14.4	6.4E-007
PP	1%C18	HP	2830601	0.051	0.026	4.5	4.2	1.00	5.4	4.2E-007

Table III-4.6 Migration of n-Octadecane into n-Octadecane

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
LPE	1%C18	OD	140301	0.138	0.072	4.7	2.1	0.97	5.4	3.1E-009
LPE	.01%C18	OD	340301	0.182	0.069	6.2	1.7	0.91	5.4	1.7E-009
LPE	5%C18	OD	540301	0.310	0.089	8.3	0.1	0.99	5.1	4.5E-008
LPE	5%C18	OD	640301	0.045	0.027	3.8	0.1	0.98	4.9	3.9E-008
BPE	10%C18	OD	840301	0.098	0.065	3.6	0.2	0.98	8.9	3.9E-008
BPE	10%C18	OD	840302	0.127	0.066	4.5	0.2	0.99	10.2	2.8E-008
BPE	1%C18	OD	940301	0.155	0.056	6.5	0.2	0.98	6.9	5.3E-009
PP	10%C18	OD	3040301	0.061	0.028	5.2	0.2	1.00	7.0	1.7E-008
LPE	1%C18	OD	140601	0.083	0.076	3.0	1.9	0.99	4.8	2.3E-008
LPE	1%C18	OD	240601	0.035	0.018	4.6	2.3	1.00	5.0	4.4E-008
LPE	.01%C18	OD	340601	0.157	0.069	5.3	1.3	0.98	5.1	3.5E-008
LPE	5%C18	OD	540601	0.325	0.085	9.0	0.1	1.00	4.8	9.6E-008
LPE	5%C18	OD	640601	0.146	0.027	11.7	0.1	1.00	4.9	1.7E-007
BPE	10%C18	OD	840601	0.099	0.065	3.7	0.2	1.00	10.0	2.2E-007
BPE	1%C18	OD	940601	0.152	0.056	6.4	0.2	1.00	7.3	1.1E-007
PP	10%C18	OD	3040601	0.071	0.027	6.1	0.2	1.00	6.7	6.8E-008

Table III-4.4 Migration of n-Octadecane into Water

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
LPE	.01%C18	AQ	380600	0.124	0.070	4.2	1.6	0.12	0.6	7.8E-013
BPE	1%C18	AQ	980600	0.167	0.057	6.7	0.2	0.06	0.5	8.2E-014
PP	1%C18	AQ	2880300	0.049	0.028	4.3	5.2	0.00	0.2	2.0E-017
PP	1%C18	AQ	2880600	0.047	0.027	4.3	5.0	0.00	0.0	1.0E-014

Table III-5.1 Migration of n-Dotriacontrane into Triglycerides

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
BPE	1%C32	CO	1610300	0.093	0.028	7.6	115.0	0.48	0.6	3.4E-012
BPE	1%C32	TB	1660300	0.045	0.028	3.8	42.6	0.70	1.3	8.4E-012
BPE	1%C32	TO	1670300	0.074	0.028	6.3	108.0	0.48	0.8	3.1E-012
LPE	1%C32	CO	1910300	0.185	0.059	7.1	5.1	0.12	1.0	1.2E-012
LPE	1%C32	TO	1970300	0.166	0.059	6.5	5.2	0.12	1.5	2.5E-012
PP	1%C32	CO	2910300	0.044	0.026	4.0	4.6	0.70	2.8	2.4E-012
PP	1%C32	TB	2960300	0.039	0.026	3.6	4.5	0.96	3.1	9.8E-012
BPE	1%C32	HB	1690400	0.029	0.029	2.8	113.0	0.75	2.2	3.7E-011
BPE	1%C32	CO	1610600	0.051	0.028	4.3	113.0	0.96	1.0	2.0E-009
BPE	1%C32	TB	1660600	0.032	0.029	2.7	116.0	0.93	0.5	2.1E-009
BPE	1%C32	TO	1670600	0.067	0.027	5.7	108.0	0.95	1.6	2.4E-009
BPE	1%C32	HB	1690600	0.019	0.028	1.7	115.0	0.95	2.0	2.9E-009
LPE	1%C32	CO	1910600	0.193	0.059	7.5	5.2	0.80	2.9	3.0E-010
LPE	1%C32	TO	1970600	0.163	0.059	6.3	5.0	0.82	4.8	4.3E-010
PP	1%C32	CO	2910600	0.046	0.027	4.1	4.1	1.00	3.3	6.3E-010
PP	1%C32	TB	2960600	0.041	0.027	3.7	5.5	0.99	3.2	1.3E-009

Table III-5.2 Migration of n-Dotriacontane into Ethanol, Ethanol/Water Mixtures and n-Octanol

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
BPE	1%C32	EN	1620300	0.051	0.028	4.2	115.0	0.17	0.3	2.3E-012
LPE	1%C32	EN	1920300	0.153	0.060	5.9	5.3	0.04	0.5	1.5E-012
PP	1%C32	EN	2920300	0.047	0.027	4.3	4.4	0.85	2.0	1.4E-011
BPE	1%C32	EN	1520600	0.187	0.064	7.1	93.0	0.76	-0.6	2.9E-009
BPE	1%C32	EN	1620600	0.076	0.030	6.3	108.0	0.86	-0.7	2.9E-009
LPE	1%C32	EN	1920600	0.190	0.060	7.5	4.2	0.63	1.0	5.8E-010
PP	1%C32	EN	2920600	0.044	0.027	4.0	5.2	0.98	1.9	2.3E-009
BPE	1%C32	.5EN	1625600	0.051	0.027	4.3	110.0	0.01	0.2	1.2E-012
LPE	1%C32	.5EN	1925600	0.189	0.059	7.4	5.2	0.00	-0.2	3.1E-014
BPE	1%C32	.95EN	1695300	0.017	0.028	1.7	115.0	0.14	0.1	1.5E-012
BPE	1%C32	.95EN	1695600	0.021	0.027	2.0	110.0	0.80	-0.5	1.9E-009
BPE	1%C32	ON	1650300	0.017	0.027	1.6	106.0	0.58	0.7	6.5E-012
LPE	1%C32	ON	1950300	0.156	0.059	6.0	5.0	0.17	2.0	2.5E-012
BPE	1%C32	ON	1650600	0.032	0.028	2.7	115.0	0.94	2.0	3.5E-009
LPE	1%C32	ON	1950600	0.091	0.058	3.9	4.9	0.80	1.9	4.7E-010

Table III-5.3 Migration of n-Dotriacontane into n-Heptane

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
BPE	1%C32	HP	1530300	0.049	0.065	1.9	96.0	0.78	7.0	7.8E-010
BPE	1%C32	HP	1630301	0.070	0.028	5.7	116.0	0.89	6.3	8.7E-010
LPE	1%C32	HP	1930301	0.190	0.061	7.5	5.2	0.73	4.5	6.9E-010
PP	1%C32	HP	2930301	0.041	0.027	4.0	5.1	1.00	5.8	1.4E-008
BPE	1%C32	HP	1530601	0.191	0.065	7.2	93.0	0.99	13.0	1.7E-007
BPE	1%C32	HP	1630601	0.069	0.028	5.7	119.0	0.99	11.0	1.6E-007
LPE	1%C32	HP	1930601	0.181	0.058	7.2	5.1	0.95	5.3	2.7E-008
PP	1%C32	HP	2930601	0.045	0.027	4.0	5.3	1.00	5.8	2.3E-007

Table III-5.4 Migration of n-Dotriacontane into Water

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ No	solv. %	Dmax cm2/s
BPE	1%C32	AQ	1680600	0.048	0.028	4.2	111.0	0.02	0.6	1.7E-015
LPE	1%C32	AQ	1980600	0.059	0.065	2.5	4.7	0.04	0.0	5.3E-013
PP	1%C32	AQ	2980300	0.046	0.027	4.2	4.5	0.00	0.0	1.0E-017
PP	1%C32	AQ	2980600	0.036	0.027	3.3	5.2	0.02	0.0	1.3E-014

Table III-6.1 Migration of BHT into Triglygerides

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	.01%BHT	CO	2010300	0.159	0.060	6.0	3.8	0.23	0.8	1.2E-011
LPE	.01%BHT	TO	2070300	0.172	0.059	6.6	3.8	0.25	0.9	1.4E-011
LPE	.01%BHT	CO	2210300	0.072	0.026	6.3	4.2	0.89	1.7	1.1E-011
LPE	.01%BHT	TB	2260300	0.045	0.026	4.0	3.1	0.75	1.2	7.3E-012
BPE	.01%BHT	CO	2310300	0.071	0.062	2.9	3.0	0.70	0.6	1.7E-010
BPE	.01%BHT	TO	2370300	0.070	0.061	3.1	3.2	0.73	1.0	2.0E-010
BPE	.01%BHT	CO	2510300	0.064	0.027	5.5	2.7	1.00	0.7	2.9E-010
BPE	.01%BHT	TB	2560300	0.061	0.027	5.3	2.9	0.98	0.3	3.4E-010
PP	.01%BHT	CO	2710300	0.052	0.027	4.7	1.7	0.30	0.6	7.3E-013
PP	.01%BHT	TB	2760300	0.039	0.027	3.5	1.8	0.75	2.1	5.5E-012
BPE	.01%BHT	HB	2590400	0.031	0.027	2.8	2.1	0.98	1.7	1.2E-009
BPE	.01%BHT	HB	2590402	0.033	0.027	2.8	2.1	0.98	1.8	1.4E-009
LPE	.01%BHT	CO	2010600	0.152	0.060	5.8	3.6	0.60	2.6	4.7E-010
LPE	.01%BHT	TO	2070600	0.166	0.060	6.3	3.7	0.61	2.3	6.5E-010
LPE	.01%BHT	CO	2210600	0.093	0.027	7.6	4.2	0.97	2.5	4.9E-010
LPE	.01%BHT	TB	2260600	0.070	0.026	5.9	4.2	0.94	1.3	4.9E-010
BPE	.01%BHT	CO	2310600	0.091	0.062	4.1	2.6	0.80	1.8	5.7E-009
BPE	.01%BHT	TO	2370600	0.077	0.062	3.2	3.0	0.76	1.8	6.7E-009
BPE	.01%BHT	CO	2510600	0.068	0.027	5.7	2.7	1.00	1.1	8.3E-009
BPE	.01%BHT	TB	2560600	0.065	0.027	5.5	2.7	0.96	0.6	8.5E-009
BPE	.01%BHT	HB	2590600	0.045	0.027	3.9	1.9	0.98	2.3	9.6E-009
LPE	.01%BHT	CO	2610600	0.056	0.027	5.2	5.5	0.97	3.7	5.5E-010
PP	.01%BHT	CO	2710600	0.046	0.027	4.2	1.9	0.87	3.8	3.2E-010
PP	.01%BHT	TB	2760600	0.035	0.027	3.3	1.7	0.88	2.7	7.0E-010

Table III-6.2 Migration of BHT into Ethanol, Ethanol/Water Mixtures, and n-Octanol

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	.01%BHT	EN	2020300	0.170	0.061	6.7	3.5	0.19	1.0	7.3E-012
LPE	.01%BHT	EN	2220300	0.063	0.027	5.2	4.4	0.85	0.6	1.9E-011
BPE	.01%BHT	EN	2320300	0.155	0.060	7.5	3.8	0.82	0.2	2.6E-010
BPE	.01%BHT	EN	2520300	0.077	0.027	6.5	2.8	1.00	0.0	3.8E-010
PP	.01%BHT	EN	2720300	0.035	0.027	3.4	1.9	0.71	0.5	6.2E-012
LPE	.01%BHT	EN	2020600	0.089	0.061	3.7	3.0	0.50	0.6	2.6E-010
LPE	.01%BHT	EN	2220600	0.067	0.027	5.8	4.5	0.95	0.6	6.6E-010
BPE	.01%BHT	EN	2320600	0.079	0.061	3.4	2.6	0.79	0.1	8.6E-009
BPE	.01%BHT	EN	2320602	0.095	0.062	3.9	2.7	0.69	0.3	7.1E-009
BPE	.01%BHT	EN	2520600	0.062	0.027	5.2	2.8	1.00	0.2	1.1E-008
BPE	.01%BHT	EN	2520602	0.072	0.029	6.0	2.7	1.00	-0.5	9.5E-009
LPE	.01%BHT	EN	2620600	0.055	0.024	5.2	5.2	0.96	0.6	6.8E-010
PP	.01%BHT	EN	2720600	0.035	0.026	3.3	1.9	0.89	1.0	9.6E-010
BPE	.01%BHT	.95EN	2595300	0.019	0.027	1.7	1.9	0.93	0.0	2.0E-010
BPE	.01%BHT	.95EN	2595600	0.020	0.027	1.7	2.0	0.93	-0.3	6.8E-009
LPE	.01%BHT	ON	2250300	0.065	0.026	5.5	3.7	0.92	1.8	1.0E-010
BPE	.01%BHT	ON	2550300	0.059	0.026	5.2	1.8	0.98	1.1	5.2E-010
LPE	.01%BHT	ON	2250600	0.040	0.026	3.5	3.7	0.94	2.2	1.6E-009
LPE	.01%BHT	ON	2250602	0.062	0.026	5.3	3.3	0.93	2.2	1.4E-009
BPE	.01%BHT	ON	2550600	0.066	0.027	5.4	2.5	0.98	2.0	1.4E-008
BPE	.01%BHT	ON	2550602	0.038	0.026	3.4	1.4	1.00	2.2	1.4E-008

Table III-6.3 Migration of BHT into n-Heptane

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	.01%BHT	HP	2030301	0.185	0.060	7.0	3.8	0.62	4.2	1.6E-008
LPE	.01%BHT	HP	2230300	0.073	0.027	6.1	4.2	0.96	3.8	2.2E-008
LPE	.01%BHT	HP	2230301	0.072	0.027	5.8	4.4	0.97	3.8	2.6E-008
BPE	.01%BHT	HP	2330301	0.077	0.062	3.2	3.9	0.82	8.0	4.2E-008
BPE	.01%BHT	HP	2530301	0.065	0.026	5.7	2.5	0.99	7.1	5.1E-008
LPE	.01%BHT	HP	2630301	0.073	0.025	6.6	5.7	0.97	6.0	2.0E-008
PP	.01%BHT	HP	2730301	0.040	0.026	3.7	1.9	0.88	5.8	1.7E-008
LPE	.01%BHT	HP	2030601	0.192	0.061	7.2	3.6	0.61	5.8	6.7E-008
LPE	.01%BHT	HP	2030602	0.134	0.061	5.4	3.4	0.58	6.5	8.2E-008
LPE	.01%BHT	HP	2130601	0.058	0.025	5.4	4.0	0.67	4.2	1.1E-007
LPE	.01%BHT	HP	2230601	0.067	0.026	5.9	4.7	0.96	4.3	1.2E-007
BPE	.01%BHT	HP	2330601	0.081	0.062	3.3	4.1	0.84	15.0	3.4E-007
BPE	.01%BHT	HP	2330602	0.089	0.063	3.5	2.8	0.78	0.0	3.4E-007
BPE	.01%BHT	HP	2330603	0.069	0.061	2.9	2.4	0.72	12.0	2.6E-007
BPE	.01%BHT	HP	2430601	0.058	0.028	5.2	1.7	0.12	13.0	2.5E-007
BPE	.01%BHT	HP	2430602	0.057	0.027	5.2	1.8	0.13	12.0	2.6E-007
BPE	.01%BHT	HP	2530601	0.072	0.027	6.4	2.8	0.97	10.4	3.7E-007
LPE	.01%BHT	HP	2630601	0.053	0.025	5.2	5.6	0.97	7.0	1.1E-007
PP	.01%BHT	HP	2730601	0.041	0.026	3.8	1.9	0.89	5.6	1.7E-007

Table III-6.4 Migration of BHT into Water

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
LPE	.01%BHT	AQ	2280300	0.069	0.028	5.8	4.0	0.32	-0.1	8.0E-013
BPE	.01%BHT	AQ	2580300	0.071	0.027	5.7	1.9	0.55	0.0	9.0E-012
PP	.01%BHT	AQ	2780300	0.042	0.027	3.8	1.7	0.16	0.1	3.0E-013
LPE	.01%BHT	AQ	2280600	0.072	0.027	5.9	3.8	0.91	0.0	6.8E-011
BPE	.01%BHT	AQ	2380600	0.160	0.062	5.9	2.3	0.50	0.0	5.6E-011
BPE	.01%BHT	AQ	2580600	0.072	0.027	6.0	2.5	0.90	-0.3	3.6E-011
PP	.01%BHT	AQ	2780600	0.045	0.027	4.3	1.8	0.60	0.1	1.0E-011

Table III-7.1 Activation Energies of Migration of n-Octadecane

Poly	Migrant	Solv	Sample Solv	D30 cm2/s	D60 cm2/s	E kJ/mol	E kcal/mol
LPE	1%C18	CO	110	1.3E-010	4.8E-009	101	24
LPE	1%C18	HP	130	1.6E-008	1.1E-007	54	13
LPE	1%C18	HP	130	1.6E-008	1.2E-007	56	13
LPE	1%C18	OD	140	3.1E-009	2.3E-008	56	13
LPE	1%C18	TO	170	1.6E-010	5.8E-009	100	24
LPE	1%C18	EN	220	1.8E-010	4.7E-009	91	22
LPE	1%C18	EN	220	1.8E-010	8.0E-009	106	25
LPE	1%C18	ON	250	2.2E-010	7.0E-009	97	23
LPE	.01%C18	CO	310	4.4E-012	1.1E-009	155	37
LPE	.01%C18	HP	330	3.7E-009	8.5E-008	88	21
LPE	.01%C18	OD	340	1.7E-009	3.5E-008	85	20
LPE	.01%C18	TO	370	6.2E-012	1.2E-009	147	35
LPE	5%C18	OD	540	4.5E-008	9.6E-008	21	5
LPE	5%C18	OD	640	3.9E-008	1.7E-007	41	10
BPE	1%C18	CO	710	1.7E-009	3.4E-008	84	20
BPE	1%C18	EN	720	5.5E-010	3.8E-008	119	28
BPE	1%C18	HP	730	4.9E-008	6.4E-007	72	17
BPE	1%C18	TO	770	1.9E-009	4.0E-008	85	20
BPE	10%C18	OD	840	3.9E-008	2.2E-007	48	12
BPE	10%C18	OD	840	2.8E-008	2.2E-007	58	14
BPE	1%C18	EN	920	6.1E-010	3.0E-008	109	26
BPE	1%C18	.5EN	925	3.4E-012	1.8E-010	111	27
BPE	1%C18	OD	940	5.3E-009	1.1E-007	85	20
BPE	1%C18	ON	950	6.5E-010	3.6E-008	112	27
BPE	1%C18	TB	960	4.4E-010	2.2E-008	109	26
BPE	1%C18	.95EN	995	4.4E-010	2.5E-008	113	27
PP	1%C18	CO	2810	2.7E-011	2.1E-009	122	29
PP	1%C18	EN	2820	9.2E-011	5.0E-009	112	27
PP	1%C18	HP	2830	5.6E-008	4.2E-007	56	13
PP	1%C18	TB	2860	4.4E-011	2.6E-009	114	27
PP	10%C18	OD	3040	1.7E-008	6.8E-008	39	9

Table III-7.2 Activation Energies of Migration of n-Dotriacontane

Poly	Migrant	Solv	Sample Solv	D30 cm2/s	D60 cm2/s	E kJ/mol	E kcal/mol
BPE	1%C32	HP	1530	7.8E-010	1.7E-007	151	36
BPE	1%C32	CO	1610	3.4E-012	2.0E-009	178	43
BPE	1%C32	EN	1620	2.3E-012	2.9E-009	200	48
BPE	1%C32	HP	1630	8.7E-010	1.6E-007	146	35
BPE	1%C32	ON	1650	6.5E-012	3.5E-009	176	42
BPE	1%C32	TB	1660	8.4E-012	2.1E-009	155	37
BPE	1%C32	TO	1670	3.1E-012	2.4E-009	186	44
BPE	1%C32	.95EN	1695	1.5E-012	1.9E-009	200	48
LPE	1%C32	CO	1910	1.2E-012	3.0E-010	155	37
LPE	1%C32	EN	1920	1.5E-012	5.8E-010	167	40
LPE	1%C32	HP	1930	6.9E-010	2.7E-008	103	25
LPE	1%C32	ON	1950	2.5E-012	4.7E-010	147	35
LPE	1%C32	TO	1970	2.5E-012	4.3E-010	144	34
PP	1%C32	CO	2910	2.4E-012	6.3E-010	156	37
PP	1%C32	EN	2920	1.4E-011	2.3E-009	143	34
PP	1%C32	HP	2930	1.4E-008	2.3E-007	78	19
PP	1%C32	TB	2960	9.8E-012	1.3E-009	137	33

Table III-7.3 Activation Energies of Migration of BHT

Poly	Migrant	Solv	Sample Solv	D30 cm2/s	D60 cm2/s	E kJ/mol	E kcal/mol
LPE	.01%BHT	CO	2010	1.2E-011	4.7E-010	103	25
LPE	.01%BHT	EN	2020	7.3E-012	2.6E-010	100	24
LPE	.01%BHT	HP	2030	1.6E-008	6.7E-008	40	10
LPE	.01%BHT	HP	2030	1.6E-008	8.2E-008	46	11
LPE	.01%BHT	TO	2070	1.4E-011	6.5E-010	107	26
LPE	.01%BHT	CO	2210	1.1E-011	4.9E-010	106	25
LPE	.01%BHT	EN	2220	1.9E-011	6.6E-010	99	24
LPE	.01%BHT	HP	2230	2.2E-008	1.2E-007	47	11
LPE	.01%BHT	HP	2230	2.6E-008	1.2E-007	43	10
LPE	.01%BHT	ON	2250	1.0E-010	1.6E-009	78	19
LPE	.01%BHT	ON	2250	1.0E-010	1.4E-009	74	18
LPE	.01%BHT	TB	2260	7.3E-012	4.9E-010	118	28
LPE	.01%BHT	AQ	2280	8.0E-013	6.8E-011	124	30
BPE	.01%BHT	CO	2310	1.7E-010	5.7E-009	98	23
BPE	.01%BHT	EN	2320	2.6E-010	8.6E-009	98	23
BPE	.01%BHT	EN	2320	2.6E-010	7.1E-009	93	22
BPE	.01%BHT	HP	2330	4.2E-008	3.4E-007	59	14
BPE	.01%BHT	HP	2330	4.2E-008	3.4E-007	59	14
BPE	.01%BHT	HP	2330	4.2E-008	2.6E-007	51	12
BPE	.01%BHT	TO	2370	2.0E-010	6.7E-009	98	23
BPE	.01%BHT	CO	2510	2.9E-010	8.3E-009	94	22
BPE	.01%BHT	EN	2520	3.8E-010	1.1E-008	93	22
BPE	.01%BHT	EN	2520	3.8E-010	9.5E-009	90	22
BPE	.01%BHT	HP	2530	5.1E-008	3.7E-007	55	13
BPE	.01%BHT	ON	2550	5.2E-010	1.4E-008	92	22
BPE	.01%BHT	ON	2550	5.2E-010	1.4E-008	92	22
BPE	.01%BHT	TB	2560	3.4E-010	8.5E-009	90	22
BPE	.01%BHT	AQ	2580	9.0E-012	3.6E-011	39	9
BPE	.01%BHT	.95EN	2595	2.0E-010	6.8E-009	99	24
LPE	.01%BHT	HP	2630	2.0E-008	1.1E-007	48	11
PP	.01%BHT	CO	2710	7.3E-013	3.2E-010	170	41

Table III-7.3 (Continued)

PP	.01%BHT	EN	2720	6.2E-012	9.6E-010	141	34
PP	.01%BHT	HP	2730	1.7E-008	1.7E-007	64	15
PP	.01%BHT	TB	2760	5.5E-012	7.0E-010	136	32
PP	.01%BHT	AQ	2780	3.0E-013	1.0E-011	98	23

may be used as the starting value in a reiterative numerical computation.

Equation (1) converges rather slowly, at small value of T, thus a sufficient number of terms must be used to avoid premature termination of the computation. At $T << 1$, approximately $3^{(-\log_{10}T)}$ terms are required to reach a reasonable precision. The following approaches may be used to simplify the computational effort depending on the conditions and ranges of applications.

Simplified Computation

At small values of $\alpha(<<1)$, a master curve of the quantity $M_t/(1+\alpha)M_\infty$, which is equal to M_{pt}/M_{so} for absorption or $M_{st}/\alpha M_{po}$ for extraction, as a function of T/α^2 may be constructed from equation (1). However, by limiting the computations to $0.1>T>0.001$, the number of terms required may be limited to about 5 at $T\sim0.1$ and about 45 at $T\sim0.001$ for reasonable accuracy. The values of $M_t/(1+\alpha)M_\infty$ at small α, but at the same T/α^2, are equal to the values calculated for large α. The results of this selective computation deviates from the more rigorous and tedious computations by about 0.001% at $T\sim0.1$, and much less than 0.001% at lower T values.

The diffusion process may be divided into three regions of T:

Region I, $T<0.1$. The system is far from equilibrium, $M_t/(1+\alpha)M_\infty$ is a function of T/α^2 only.

Region II, $5>T>0.1$. The system is approaching equilibrium and detailed computation must be carried out for different α values (only 2 to 6 terms are required for equation (1) in this region). For $\alpha<<1$ and $T/\alpha^2>10^3$, $M_t/(1+\alpha)M_\infty = 1 - \alpha/(\pi T)^{1/2}$ before reaching equilibrium.

Region III, $T>5$. For all practical purposes, equilibrium has been reached with the deviation $\delta = 1-M_t/M_\infty \leq 10^{-T}$, where $M_\infty = M_{so}/(1+\alpha)$ for

the case of absorption and $M_\infty = M_{po}\alpha/(1+\alpha)$ for the case of extraction. For $\alpha<1$, equilibrium may be reached much earlier.

Computation for Migration into Infinite Media

When $\alpha\to\infty$, M_t/M_∞ approaches a limit, and equation (1) can be reduced to a function of T only:

$$M_t/M_\infty = 1 - 2 \sum_{n=1}^{\infty} \frac{1}{q_n^2} \exp(-q_n^2 T) \qquad (2)$$

where $q_n = (n-1/2)\pi$. For $T<0.1$, M_t/M_∞ is a linear function of $T^{1/2}$.

$$M_t/M_\infty = 2(T/\pi)^{1/2} = 1.128379\ T^{1/2} \qquad (3)$$

Deviations of equation (3) from equation (2) is less than 10^{-10} at $T<0.05$, about 10^{-6} at $T = 0.1$, about 5×10^{-4} at $T = 0.2$ and becomes much greater than 0.01 at $T = 0.3$ or higher.

Alternate Approximation

An alternative form of the solution[7]

$$M_t/M_\infty = (1+\alpha)\ [1 - e^{T/\alpha^2}\ \mathrm{erfc}(T^{1/2}/\alpha)], \qquad (4)$$

may be used in some cases and is relatively simple to compute. One of the rational approximations[8] for the error function yields the following

$$M_t/(1+\alpha)M_\infty = 1 - \sum_{n=1}^{5} a_n \tau^n + \varepsilon \qquad (5)$$

where $\tau=1/(1+0.3275911\ T^{1/2}/\alpha)$, $a_1=0.254829592$, $a_2=-0.28449636$, $a_3=1.421413741$, $a_4=-1.453152027$, $a_5=1.061405429$, and $|\varepsilon|<\omega 1.5 \times 10^{-7}$.

At $\alpha<<1$, results computed from equation (2) or (3) deviates less than 0.0001 from that of equation (1) at $T/\alpha^2<5$ or at $M_t/(1+\alpha)M_\infty<0.75$. Maximum deviation of 0.0035 occurs at $T/\alpha^2\sim500$ or at $M_t/(1+\alpha)M_\infty\sim0.97$. Therefore, equation (4) or (5) may be used to generate the master curve for equation (1) at $T<0.1$ (Region I). However equations (4) or (5) do not yeild any information about the region approaching equilbrium at larger values of α, and hence should be used with discretion.

By combining Equation (4) or (5) at T<0.1 (Region I) and Equation (1) at T>0.1 (Region II and III), computational requirements for the solution of the diffusion equation between a plane sheet and a well stirred liquid may be reduced to a minimum.

Diffusion coefficient at any point may be estimated from the above computation method by means of regression.

Effect of Swelling

The diffusion coefficients in the tables are calculated based on the original measured thickness of the sample, which is also given in the tables. The final sample is usually swollen with solvent. For volatile solvents, the absorbed solvent will leave the polymer soon after the sample is taken out of the extracting solvent. In these cases, the final sample weight is determined immediately after the surface of sample has been wiped free of the solvent. The dimensions of the final sample are generally not measured, however they may be estimated from the amount of solvent absorption by assuming an isotropic expansion. The diffusion coefficient may be adjusted to reflect the increase in the thickness as follows:

$$D = D_o \left(\frac{L}{L_o}\right)^2 = D_o \left(\frac{V}{V_o}\right)^{2/3}$$
$$= D_o \left[1 + \frac{\delta_f}{1-\delta_f} \cdot \frac{\rho_o}{\rho_s}\right]^{2/3}$$

where $\delta_f = (W_f - W_o)/W_f$. D, L, V, M and p are the diffusion coefficient, thickness, volume, weight and density respectively. The subscripts o, f, and s denote the original polymer, final polymer and solvent respectively. The sum of fractional weight increase δ_f and the fractional decrease in weight due to the migrant loss is given also in the table and indicates the weight percent of solvent content in the final sample. Therefore, the diffusion coefficients based on the final sample thickness

are increased from those based on the original thickness by approximately the same order of magnitude as the increases in weight.

Table II-1

Characteristics of Polyolefin Samples

		Linear Polyethylene NBS-SRM 1475	Branched Polyethylene NBS-SRM 1476	Isotactic Polypropylene Pro-fax 6301*
Molecular Weights	M_n	18,310 (GPC)		
	M_w	53,070 (GPC)		290,000
	M_w	52,000 (LS)		
	M_w/M_n			11
Limiting Viscosity Number [n],dl/g	CN	0.890	0.8132	
	TCB	1.010	0.9024	
	DHN	1.180	1.042	2.1
Melt Flow Rate, g/10 min		2.07	1.19	
Density, g/cm^3		0.97844	0.9312	
Isotacticity, %				95-96

GPC -- Gel Permeation Chromatography

LS -- Light Scattering

CN -- 1-chloronaphthalene

TCB -- 1,2,4-trichlorobenzene

DHN -- decahydronaphthalene (Decalin)

t [n] = 130°C for polyethylenes, 135°C for polypropylene

Melt Index by Procedure A, ASTM Method D 1238-65T, Test Condition D, 190°C, load 325 g for SRM 1475 and 1260 g for SRM 1476.

Density by ASTM Method D 1505-67; sample prepared by Procedure A, ASTM Method D 1928-68.

Isotacticity is determined as fractional insoluble in Decalin at room temperature after the entire sample has been dissolved at 160°C and allowed to cool.

*Certain commercial materials and equipment are identified in this papger to adequately specify the experimental procedure. This identification does not imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the material or equipment identified is necessarily the best available for the purpose.

Table II-2

Characteristics of Ethylene-Vinyl Acetate Copolymers

Designation	Vinyl Acetate Content %	M_n	M_n	Melt Index g/10 min	Density g/cm^3
Petrothene NA294-00	5.1	15000	89300	1.9	0.925
Ultrathene UE657-00	13.4	18700	103000	0.46	0.935

Table II-3

Characteristics of Radioactive Tracers

	μC_i/mg	ng/25 dpm
n-$C_{18}H_{38}$-1-^{14}C	86.0	0.13
	13.3	0.83
n-$C_{32}H_{66}$-16,17-^{14}C	45.5	0.25
3,5-di-tert-butyl-4 hydroxytoluene-7-^{14}C (BHT)	57.9	0.19

Table II-4

Solvent $X10^3$	Temperature $X10^1$	Method $X10^0$
10, Corn Oil (CO)	24, 24°C	0, Limited Solvent Volume (L)
20, Ethanol (EN)	30, 30°C	1, Unlimited Solvent Volume (U)
	40, 40°C	2-8, Duplicate (or Renewed Extractions)
21, 10% Ethanol (.1 EN)	60, 60°C	9, Absorption Experiment (A)
23, 30% Ethanol (.3 EN)		
25, 50% Ethanol (.5 EN)		
27, 70% Ethanol (.7 EN)		
29, 90% Ethanol (.9 EN)		
30, n-Heptane (HP)		
40, n-Octadecane (OD)		
50, n-Octanol (ON)		
60, Tributyrin (TB)		
70, Trioctanoin (TO)		
80, Water (AQ)		
90, HB307 (HB) Synthetic Triglyceride Mixture		
95, 95% Ethanol (.95 EN)		

Letters in paratheses are abbreviations used in tables.

Table II-5

Sample Code $\times 10^5$	Polymer	Migrant	Nominal Migrant Conc.,%	Sp. Act. μCi/ g. Polymer	Thickness cm
1	LPE	C18	0.64	2.1	0.072
2	LPE	C18	0.63	2.2	0.019
3	LPE	C18	0.013	1.6	0.070
4	LPE	C18	0.01	0.96	0.020
5	LPE	C18	5.2	0.14	0.084
6	LPE	C18	5.5	0.13	0.027
7	BPE	C18	0.85	0.020	0.064
8	BPE	C18	9.8	0.23	0.066
9	BPE	C18	0.85	0.17	0.057
11	LPE	C18	0.009	1.1	0.263
13	BPE	C18	0		0.064
14	LPE	C18	0		0.064
15	BPE	C32	1.86	93.	0.064
16	BPE	C32	2.26	113.	0.028
17	BPE	C32	0		
18	LPE	C32	0		
19	LPE	C32	1.0	5.2	0.059
20	LPE	BHT	0.0062	3.6	0.060
21	LPE	BHT	0.0069	4.0	0.025
22	LPE	BHT	0.0072	4.2	0.027
23	BPE	BHT	0.0052	3.0	0.061
24	BPE	BHT	0.0030	1.8	0.028
25	BPE	BHT	0.0045	2.6	0.027
26	LPE	BHT	0.0095	5.5	0.025
27	PP	BHT	0.0029	1.8	0.027
28	PP	C18	0.82	4.9	0.027
29	PP	C32	0.97	5.3	0.027
30	PP	C18	6.8	0.16	0.028
31	E-5% VA	BHT	0.0091	5.3	0.029
32	E-13% VA	BHT	0.0057	3.3	0.069

References

1. Sanchez, I. C., Chang, S. S., McCrackin, F. L. and Smith, L. E., "An Evaluation of Existing Models Describing the Migration of Additives in Polymers," NBSIR 78-1499, 1978.

2. Smith, L. E., Sanchez, I.C., Chang, S. S. and McCracking, F. L., "Models for the Migration of Paraffinic Additives in Polyethylene," NBSIR 79-1598, 1979.

3. Smith, L. E., Sanchez, I. C., Chang, S. S., McCrackin, F. L., and Senich, G. A., "Models for the Migration of Additives in Polyolefins," NBSIR 79-1779, 1979.

4. Smith, L. E., Chang, S. S., McCrackin, F. L., Sanchez, I. C. and Senich, G. A., "Models for the Migration of Additives in Polyolefins," NBSIR 80-1999, 1980.

5. Smith, L. E., Chang, S. S., McCrackin, F. L., Senich, G. A. and Wang, F. W., "Models for the Migration of Low Molecular Weight Additives in Polyolefins," NBSIR 81-2264, 1981.

6. Smith, L. E., Chang, S. S. and Senich, G. A., "Migration of Low Molecular Weight Additives in Polymers," NBSIR 81-2314, 1981.

7. Crank, J. "The Mathematics of Diffusion," Oxford University Press, 1975.

8. Abramowitz, M. and Stegun, L. A., "Handbook of Mathematical Functions," AMS 55, National Bureau of Standards, GPO, 1964.

III. Results of Polyolefin Extraction Experiments

The results of extraction experiments are summarized in Table III.1 through III.3 for the extraction of n-octadecane, n-dotriacontane and BHT by triglycerides, ethanol, n-octanol, ethanol/water mixtures, n-heptane, n-octadecane, and water.

The tables provide information on the test pieces as to their weight, thickness L, exposed area A, specific activity of polymer, amount extracted at the end of experiment M_f/M_o, the amount of solvent retained in the final sample and the observed maximum of the diffusion coefficient.

The value for M_f/M_o in the tables is the final fraction of total additives migrated at the end of the experiment. It may be either an equilibrium value or a non-equilibrium value after a long time (6 months to one year) lapse. In the case of BHT experiments, most of the M_f values for migration into good solvents denote the available fraction of BHT in the sample, which varies with the conditions underwhich the sample was prepared. Therefore, in calculating diffusion coefficients for samples containing BHT, an adjusted M_o is assigned to each sample according to the equilibrium (M_f/M_o) values observed in the good solvents. For the case of n-$C_{32}H_{66}$ in polypropylene or other samples which exhibit surface blooming of migrants, the total amount of migrant is also adjusted for the amount of migrant on the surface, before diffusion coefficients calculating from it.

Tables III-1 through III-3 summarize the experimental results arranged by migrant or additive and then according to the type of polymer, additive concentration, sample thickness, and, finally, solvents and temperature. In order to provide easy cross-references, Tables III-4

through III-6 summarize the experimental results which are arranged first by solvent and then by additive and other parameters.

The activation energies, E, calculated by a simple Arrhenius equation:

$$D = A \exp(-E/RT)$$

are given in Table III-7.

IV. Loss of BHT from Polymers in Ambient Atmosphere

ADL, Inc. had reported through private communications concerning the high volatility of BHT from their samples. When we examined our observed total BHT contents from various experiments over a 1 1/2 year period on a branched polyethylene sample, code 25, containing 45 ppm of BHT, we found a rather noticeable trend of decreasing radioactivities as a function of starting date of the experiment, Figure IV-1, although the sample plaque was always wrapped in aluminum foil except during short periods when pieces were cut from the plaque.

The volatility of BHT is further indicated by the following experiment. A piece of E-13% VA copolymer containing 60 ppm of BHT (sample code 32), 61 mg in weight with about 2 cm^2 of surface area, was placed in a sealed 20 ml vial. The bottom of the vial was kept at 30°C and the vial cap at 22-23°C. After 63 hours it was found that the aluminum cap liner had a radioactivity of 0.51% of the test piece and the glass wall of the vial had a radioactivity of 0.95% of the test piece. Thus in a relatively short period, 1.5% of the BHT was sublimed from the test piece at rather low temperatures in a closed vessel.

A further test was performed on both sample plaques 25 and 32. Four pieces were cut from each of the sample plaques. These four pieces were subjected to the following tests:

(A) The test piece was dissolved in o-xylene to check the current specific activity.

(B) The test piece was extracted immediately by ethanol at 60°C for three days. The residual specific activity and the activity of the extract were recorded.

(C) The test piece was suspended in a ventilation hood at room temperature for three days before procedure (B) was performed.

(D) The test piece was placed in a vial. Forced air was blown into the vial for three days at room temperature before procedure (B) was performed.

The results of these tests are presented in Table II-1. The test pieces A and B were used as controls. Apparently 30 to 50% BHT is lost from thin sheets of BPE or E-VA copolymer in mobile air at room temperature for three days. The specific activity of sample code 25, BHT in BPE, at the time of these tests was only 50% of the original specific activity of 2.8 μCi/g polymer, determined 16 months earlier.

These experiments and our prior experience indicate that: (1) the amount of additive remaining in the polymer after processing to produce plaques is a fraction of the additive mixed into the raw polymer, (2) for certain reactive additives, only a fraction of additive in the polymer may be extractable, the rest may be chemically bound to the polymer, (3) the total activity of the test pieces should be checked for each experiment not only to measure the uniformity of the additive concentration but also to measure the change in additive content as a function of time. Therefore reports which the results are normalized to the amount of additive supposely added to the polymer or to the total amount of additive present in the polymer when it was manufactured, without paying further attention to the amount of additive either reacted or lost, may yield seriously incorrect kinetics of migration.

Table IV-1

Sample Code	Test Piece	Specific Activities, μCi/g polymer Residue	Total	Percent of Original Activity (Average of A + B)
25 BHT in BPE	A	--	1.28	100
	B	0.042	1.30	100
	C	0.053	.93	72
	D	0.052	.89	69
32 BHT in E-13% VA	A	--	3.29	100
	B	0.077	3.45	100
	C	0.081	2.18	65
	D	0.068	1.49	44

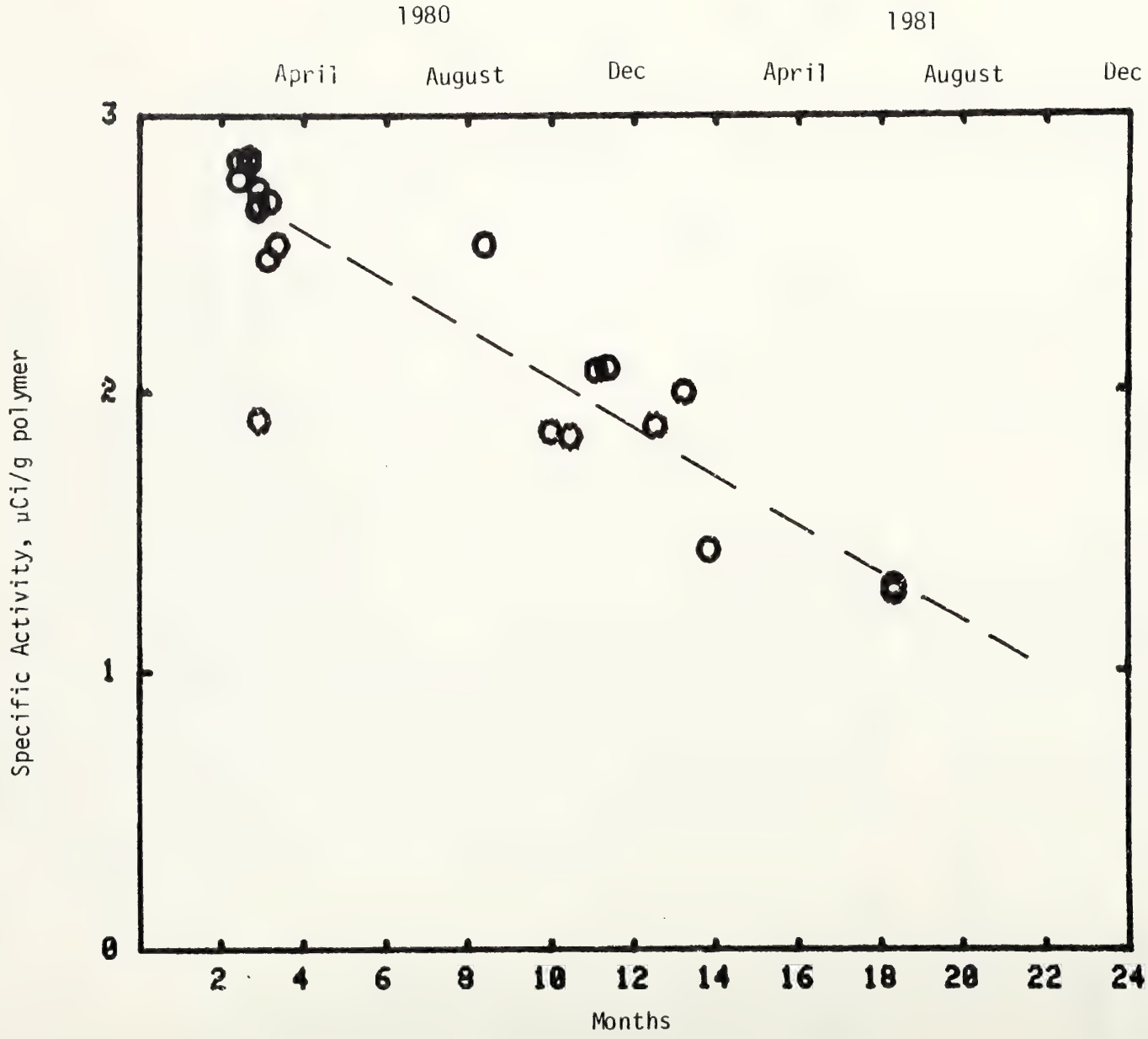


Figure IV-1

Loss of BHT from Sample 25, BHT/BPE

V. Migration of BHT from Ethylene-Vinyl Acetate Copolymers

Ethylene-vinyl acetate (E-VA) copolymers of relatively low vinyl acetate contents have been used in increasing quantities in recent years as food-contact polymer films. The migration of the antioxidant BHT from two copolymers having 5 and 13% vinyl acetate content into corn oil, anhydrous ethanol, 95% ethanol, water and n-heptane was observed with ^{14}C-labeled BHT. The characteristics of these polymers were shown earlier in Table I-2. The characteristics of the additive BHT were presented earlier in Table I-3. The sample plaques were prepared in similar manner to those of polyethylene and polypropylene samples described earlier, except that lower molding temperatures were used for the E-VA copolymers. The E-5% VA and E-13% VA samples were designated as plaque 31 and 32 with thickness of 0.027 and 0.068 cm and BHT contents of 9 and 57 PPM, respectively.

The results for individual extraction experiments are summarized in Table V-1. E-VA copolymers absorb a fair amount of solvents as shown in the table. The listed values are fractional weights of solvent contained in the final sample. Thus for experiment 3230600, the final sample contained n-heptane amounting to about 120% of the original weight of the polymer. The 12% corn oil content for sample 3210600 is higher than all other corn oil experiments.

The results of all extraction experiments for individual E-VA copolymers are shown graphically in Figures V-1.1 through V-1.4 for the migration of BHT from E-5% VA at 30 and 60°C, and from E-13% VA at 30 and 60°C, respectively. There are three illustrations for each figure, i.e., (A) M_t/M_o is plotted against t/L^2 in a log-log plot to indicate the migration behavior over several orders of magnitudes in both M_t/M_o and time, (B) M_t/M_o is plotted against $t^{1/2}/L$ for the short time region

to indicate the behavior observed during fast extractions, and (C) M_t/M_o is plotted against $t^{1/2}/L$ for the entire length of time of experiments.

From both Tables V-1 and Figures V-1, the residual BHT content in the 5% vinyl acetate copolymer samples, code 31, at the end of extration are seen to vary from 7 to 12%. It is estimated from graphical extrapolation that approximately 7-8% of the original BHT content is not extractable even by good solvents, such as n-heptane. Almost all of the BHT content in the 13% vinyl acetate copolymer is extractable. The 5% water content in 95% ethanol has no noticeable effect on the BHT extractability for the copolymers. No partitioning of BHT was observed between the copolymers and solvents such as n-heptane, corn oil, anhydrous ethanol and 95% ethanol, due to the near-complete of extraction of all available BHT from the copolymers by these solvents.

Figures V-2.1 through 5 show the migrational behavior of BHT from E-VA copolymers into various solvents, n-heptane, corn oil, ethanol, 95% ethanol and water. These illustrations offer comparisons of behavior among different E-VA copolymers and/or at different temperatures of extraction.

In a more concise comparison of this behavior, the apparent maximum diffusion coefficients of the swollen polymers are listed in Table V-2 together with the activation energies for diffusion. In all cases except water, the diffusion coefficient for the 13% vinyl acetate copolymer is about 2 to 3 times greater than that for the 5% copolymer. Increasing in the temperature from 30 to 60°C generally increases the diffusion coefficient by 10 to 20 fold, although the changes for the solvent n-heptane are only on order of 4 to 6.

The diffusion coefficients in 95% ethanol are only slightly less than those for anhydrous ethanol, about 10-15% less for 5% vinyl acetate copolymers and about 25-45% less for 13% copolymer. Both diffusion

coefficients for experiments in anhydrous ethanol and 95% ethanol are greater than those for corn oil by similar magnitudes.

The migrational behavior of BHT from the two E-VA copolymer into water is rather unusual, as can be seen in figure V-2.5. The log (M_t/M_o) versus log (t/L^2) representation in Figure V-2.5 is changed for Figures V-3.B and V-3-C into the more familiar M_t/M_o versus $t^{1/2}$ representation. Figure V-3-B is the short-time portion of Figure V-3-C which covered the entire time scale of experiment. These results indicate that the migration of BHT from E-VA copolymer into water occurs in two distinct stages, and that in contrast to the observations for other solvents, the diffusion coefficients of BHT from E-13% VA copolymer are slower than those from E-5% VA copolymer in the first stage. In the second stage the diffusion coefficients from E-13% VA are apparently approaching those from E-5% VA and can even surpass the latter when the time of experiment is lengthened to allow equilibrium extraction.

In the first stage, 10-50 hours, approximately 15% of the BHT from E-5% VA copolymer and about 1% of the BHT for E-13% VA copolymer, were extracted by water before the release of BHT levels off into a second stage behavior. It has not been determined whether the second stage of extraction, with its distinctly different diffusion coefficient, is due to the distribution of BHT in phase-separated regions of the copolymers or due to the reaction of water and BHT over prolonged periods.

Another plausible explantion for the two stage behavior would be surface blooming, or a very high migrant concentration near the surface layer, although the time lapse of 10 to 50 hours seems to be longer than usually needed to remove migrant from the surface or surface layer. By extending the second stage behavior to t=0, one may estimate from

Figure V-3-B that there might exist surface blooming of BHT amounts to about 7.5 and 11% for the E-5% VA copolymer and 0.6 and 0.57% for the E-13% VA copolymer, for 30 and 60°C experiments, respectively.

The diffusion coefficients presented in Table V-2 were calculated by first adjusting the original loading, M_0, to the available BHT, M_0^*, when necessary. The first stage diffusion coefficients were calculated based on the above mentioned percentages for M_∞/M_0^*. By substracting the first stage M_∞, normalizing and then applying equilibrium partitioning when applicable, the second stage difficient coefficients were estimated.

Equilibrium partitioning of BHT between the copolymers and solvents was observed only for the case of E-5% VA and water at 60°C. In all other experiments with water, a time lapse of six months was not long enough to establish an equilibrium conditions.

Table V-1.1 Migration of BHT from E-5% VA Copolymer

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
EVA.05	BHT	CO	3110300	0.033	0.030	2.8	4.2	0.88	2.8	1.5E-009
EVA.05	BHT	CO	3110600	0.032	0.028	2.8	4.7	0.88	3.6	2.3E-008
EVA.05	BHT	EN	3120300	0.030	0.028	2.8	4.7	0.89	0.5	1.9E-009
EVA.05	BHT	EN	3120600	0.035	0.029	2.8	5.7	0.90	0.7	3.7E-008
EVA.05	BHT	HP	3130300	0.032	0.029	2.8	5.0	0.91	12.4	1.4E-007
EVA.05	BHT	HP	3130600	0.030	0.029	2.9	5.3	0.92	15.2	5.7E-007
EVA.05	BHT	.95EN	3195300	0.064	0.027	5.6	3.8	0.93	0.5	1.7E-009
EVA.05	BHT	.95EN	3195600	0.062	0.028	5.2	3.9	0.92	1.0	3.2E-008
EVA.05	BHT	AQ	3180300	0.036	0.030	2.6	3.4	0.34	0.0	4.6E-011 9.6E-013
EVA.05	BHT	AQ	3180600	0.028	0.030	2.4	3.8	0.71	0.3	5.0E-010 2.8E-011

Table V-1.2 Migration of BHT from E-13% VA Copolymer

Polymer	Migrant	Solvent	RUN #	WT. g	L cm	A cm2	mmCi/ g.poly	Mf/ Mo	solv. %	Dmax cm2/s
EVA.13	BHT	CO	3210300	0.137	0.072	4.7	3.7	1.00	4.3	3.7E-009
EVA.13	BHT	CO	3210600	0.121	0.067	4.5	3.2	1.00	12.0	4.9E-008
EVA.13	BHT	EN	3220300	0.158	0.072	5.4	3.4	1.00	2.6	1.0E-008
EVA.13	BHT	EN	3220600	0.136	0.071	4.6	3.5	1.00	4.0	1.0E-007
EVA.13	BHT	HP	3230301	0.130	0.068	4.7	3.2	0.99	19.0	3.0E-007
EVA.13	BHT	HP	3230601	0.127	0.070	4.5	3.6	0.99	58.0	1.8E-006
EVA.13	BHT	.95EN	3295300	0.157	0.067	5.8	3.3	0.99	1.6	5.5E-009
EVA.13	BHT	.95EN	3295600	0.156	0.066	5.6	3.2	0.99	3.0	7.5E-008
EVA.13	BHT	AQ	3280300	0.147	0.068	5.5	3.1	0.06	0.2	7.0E-013 2.3E-013
EVA.13	BHT	AQ	3280600	0.123	0.068	4.4	3.0	0.37	0.1	3.4E-012 1.0E-011

Table V-2

Diffusion Coefficients and Activation Energies of
Migration of BHT from Ethylene-Vinyl Acetate Copolymers into Various Solvents

	D_{max} (10^{-8} $cm^2 s^{-1}$)				E	
	30°C		60°C		kJ mol^{-1}	
Solvent	E5%VA	E13%VA	E5%VA	E13%VA	E5%VA	E13%VA
n-Heptane	14	30	57	180	39	51
Corn Oil	0.15	0.37	2.3	4.9	76	72
Ethanol	0.19	1.0	3.7	10	83	65
95% Ethanol	0.19	0.55	3.2	7.5	82	73
Water - 1st Stage	0.0046	0.00007	0.005	0.00034	67	44
2nd Stage	0.000096	0.000023	0.0028	0.0010	94	106

Figure V-1.1-A, B, C Migration of BHT from E-5% VA Copolymer at 30°C

Figure V-1.2-A, B, C Migration of BHT from E-5% VA Copolymer at 60°C

Figure V-1.3-A, B, C Migration of BHT from E-13% VA Copolymer at 30°C

Figure V-1.4-A, B, C Migration of BHT from E-13% VA Copolymer at 60°C

Legends for Figure V-1.1

Corn Oil

Ethanol

95% Ethanol

n-Heptane

Water

Figure V-1.1-A

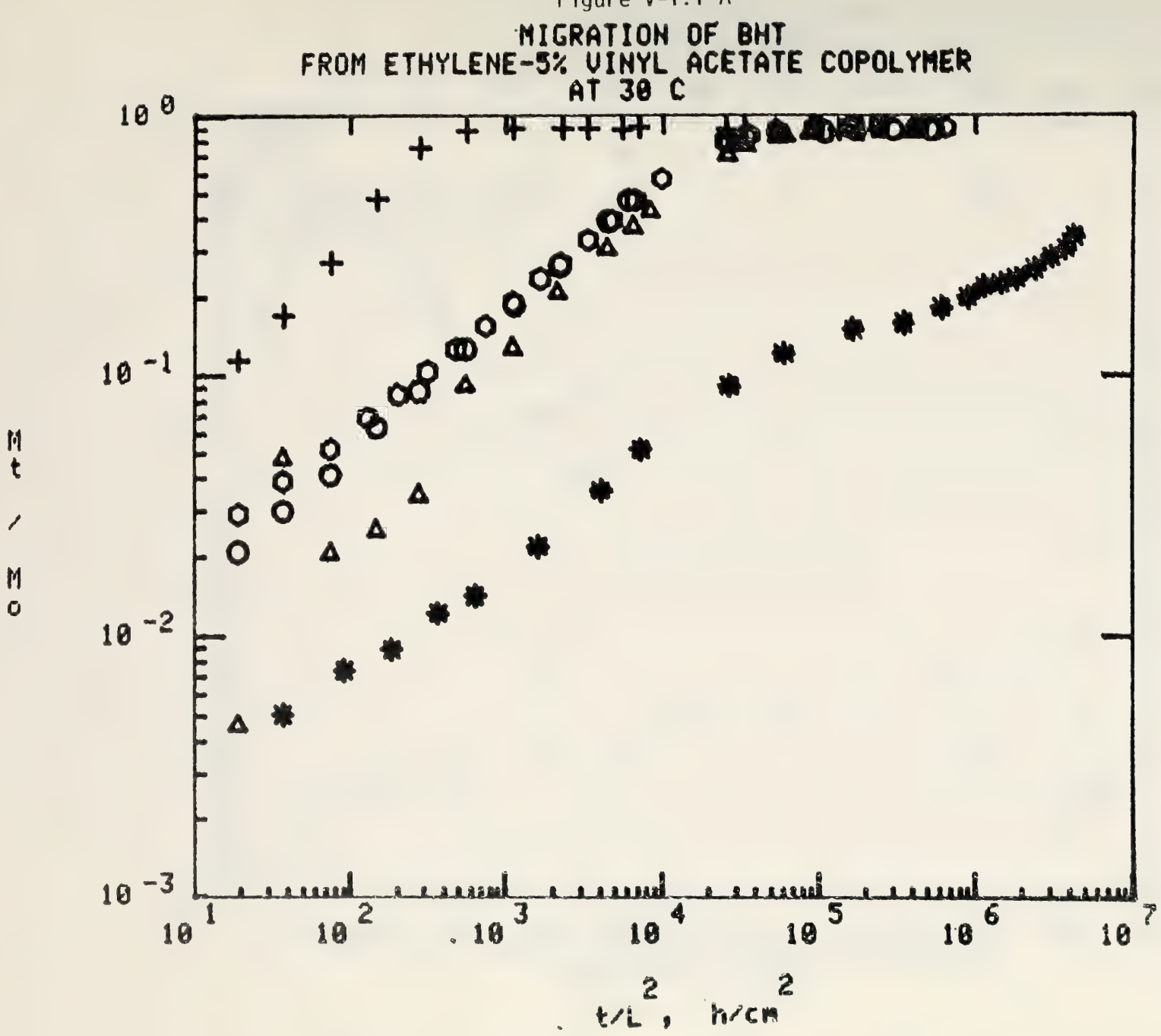

MIGRATION OF BHT
FROM ETHYLENE-5% VINYL ACETATE COPOLYMER
AT 30 C
10 0
10 -1
10 -2
10 -3
M t / M o
10 1
10 2
10 3
10 4
10 5
10 6
10 7
t/L 2 , h/cm 2

Figure V-1.1-B

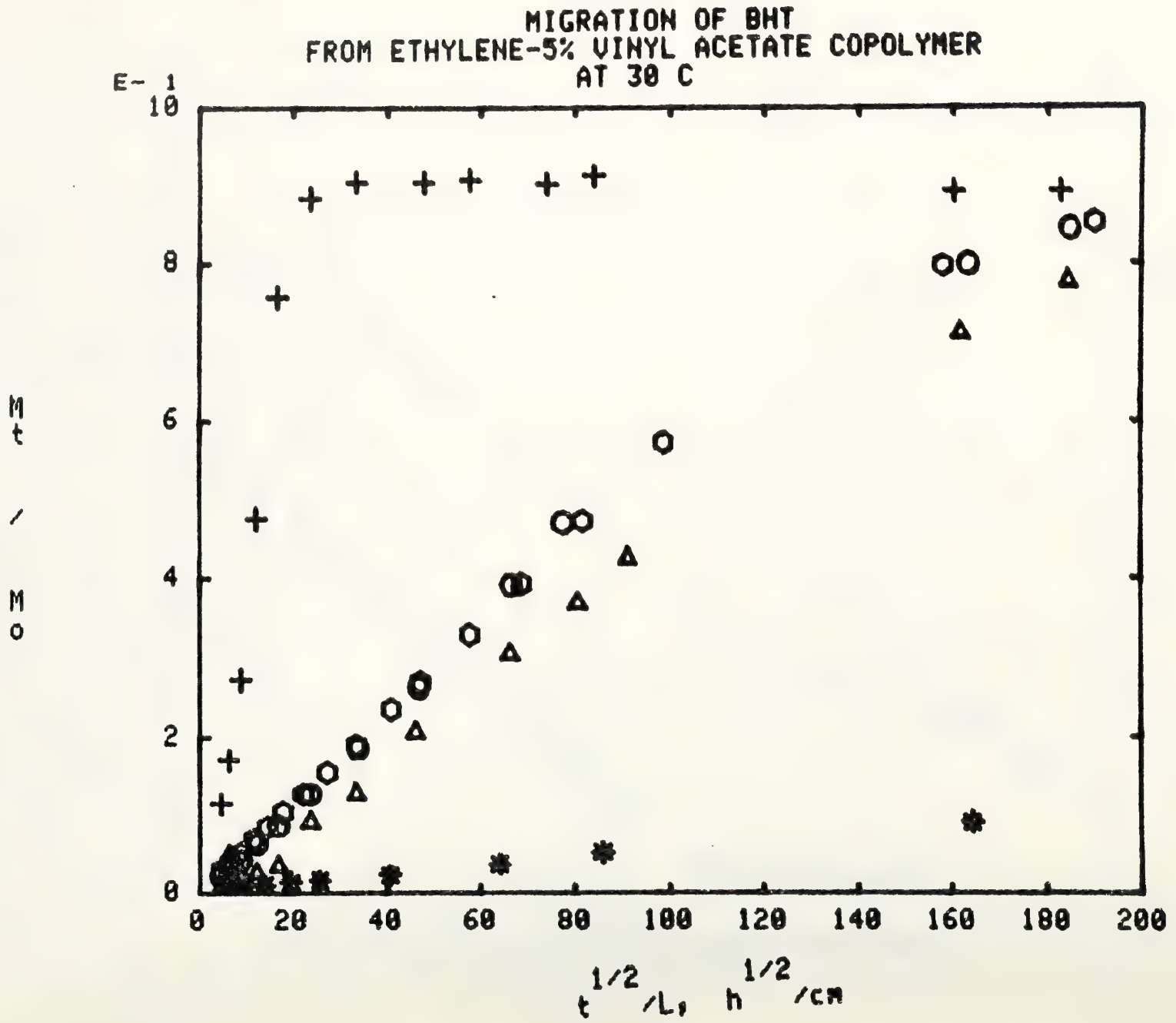

MIGRATION OF BHT
FROM ETHYLENE-5% VINYL ACETATE COPOLYMER
AT 30 C
E- 1
10
8
6
4
2
0
M
t
/
M
o
0
20
40
60
80
100
120
140
160
180
200
t 1/2 /L, h 1/2 /cm

Figure V-1.1-C

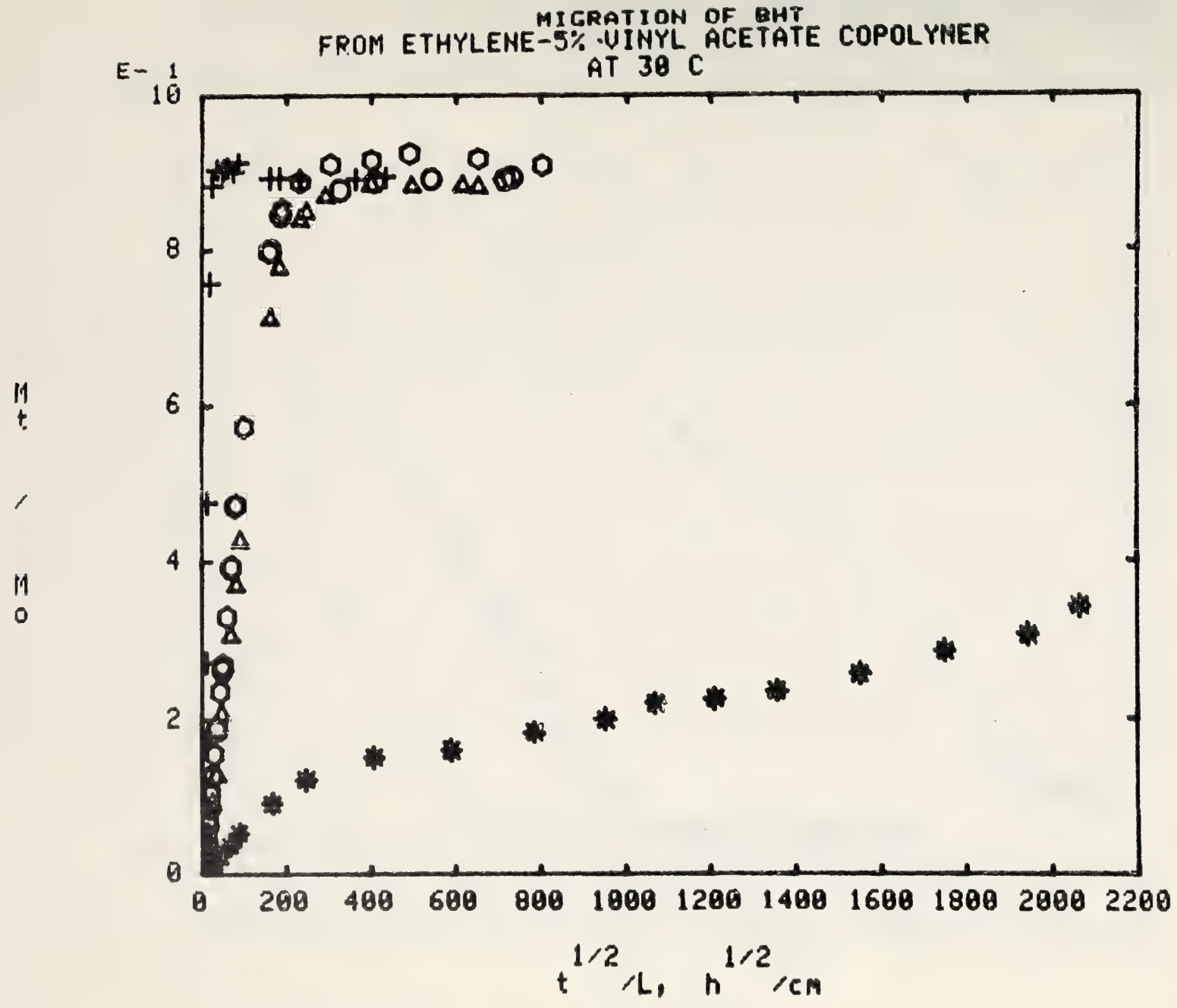

MIGRATION OF BHT
FROM ETHYLENE-5% VINYL ACETATE COPOLYMER
AT 30 C
E- 1
10
8
6
4
2
0
Mt / Mo
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
t 1/2 /L, h 1/2 /cm

Figure V-1.2-A

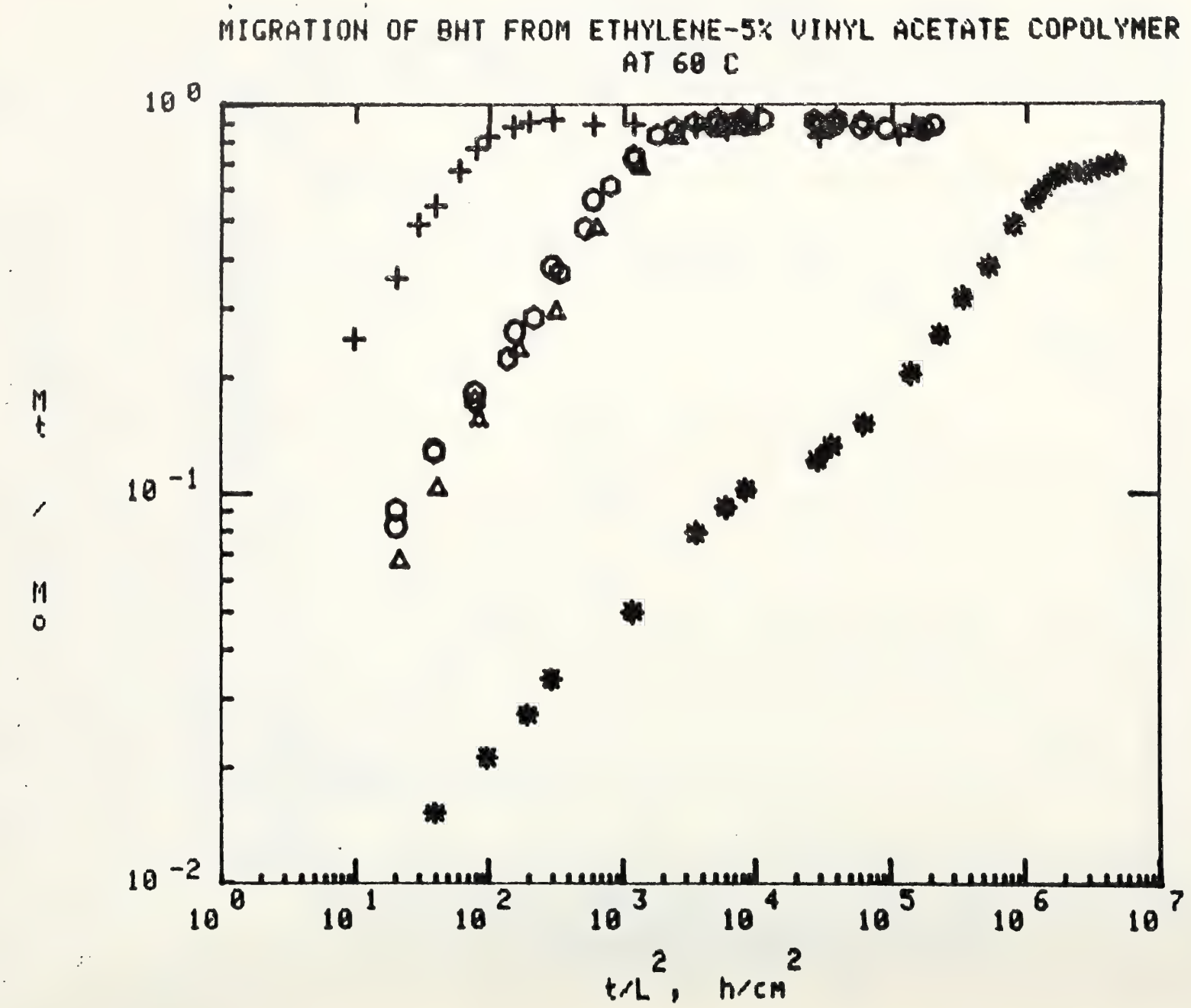

MIGRATION OF BHT FROM ETHYLENE-5% VINYL ACETATE COPOLYMER
AT 60 C
10 0
10 -1
10 -2
M t / M o
10 0
10 1
10 2
10 3
10 4
10 5
10 6
10 7
t/L 2 , h/cm 2

Figure V-1.2-B

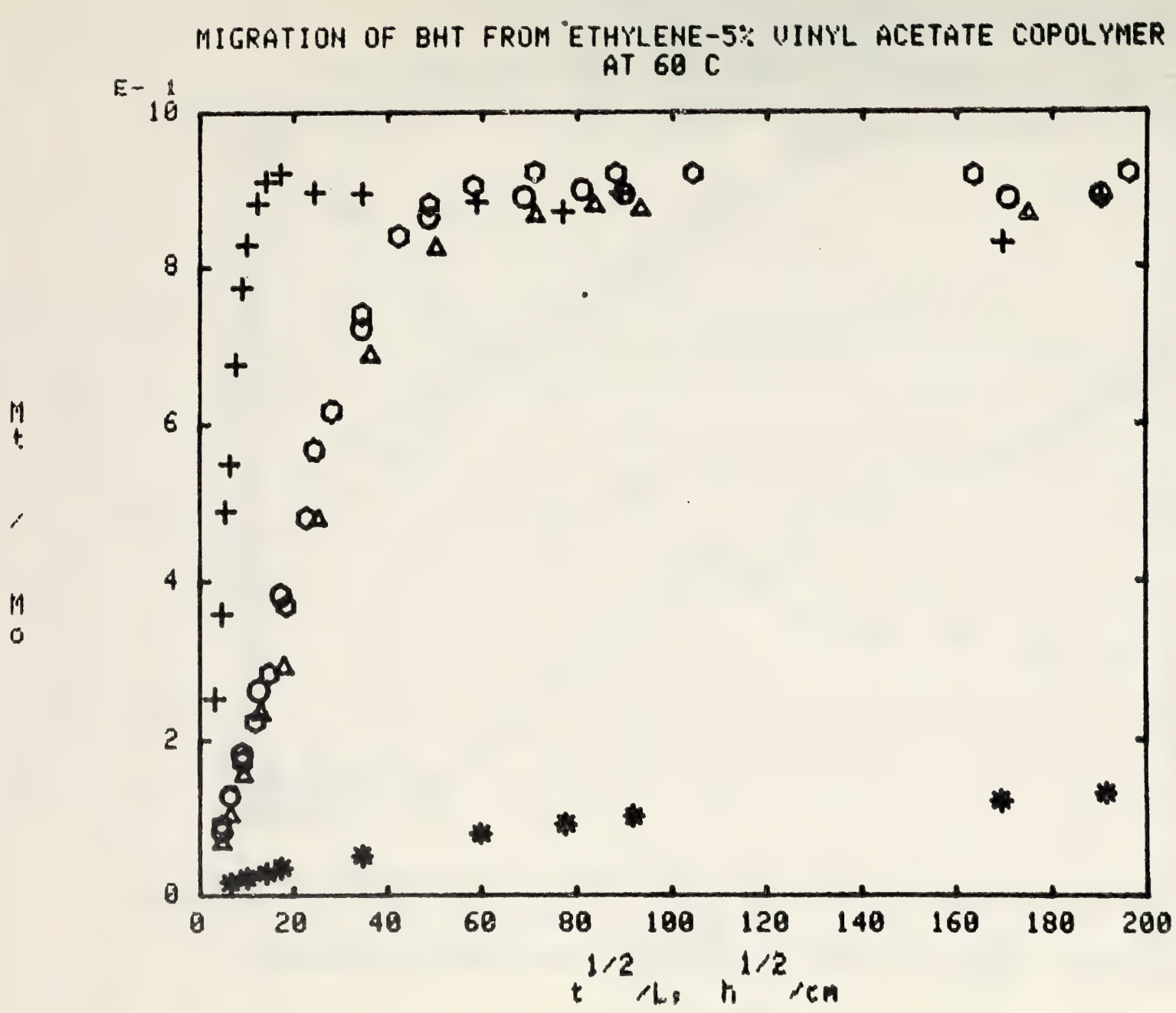

MIGRATION OF BHT FROM ETHYLENE-5% VINYL ACETATE COPOLYMER
AT 60 C
E- 1
10
8
6
4
2
0
M
t
/
M
o
0
20
40
60
80
100
120
140
160
180
200
1/2
t /Ls
1/2
h /cm

Figure V-1.2-C

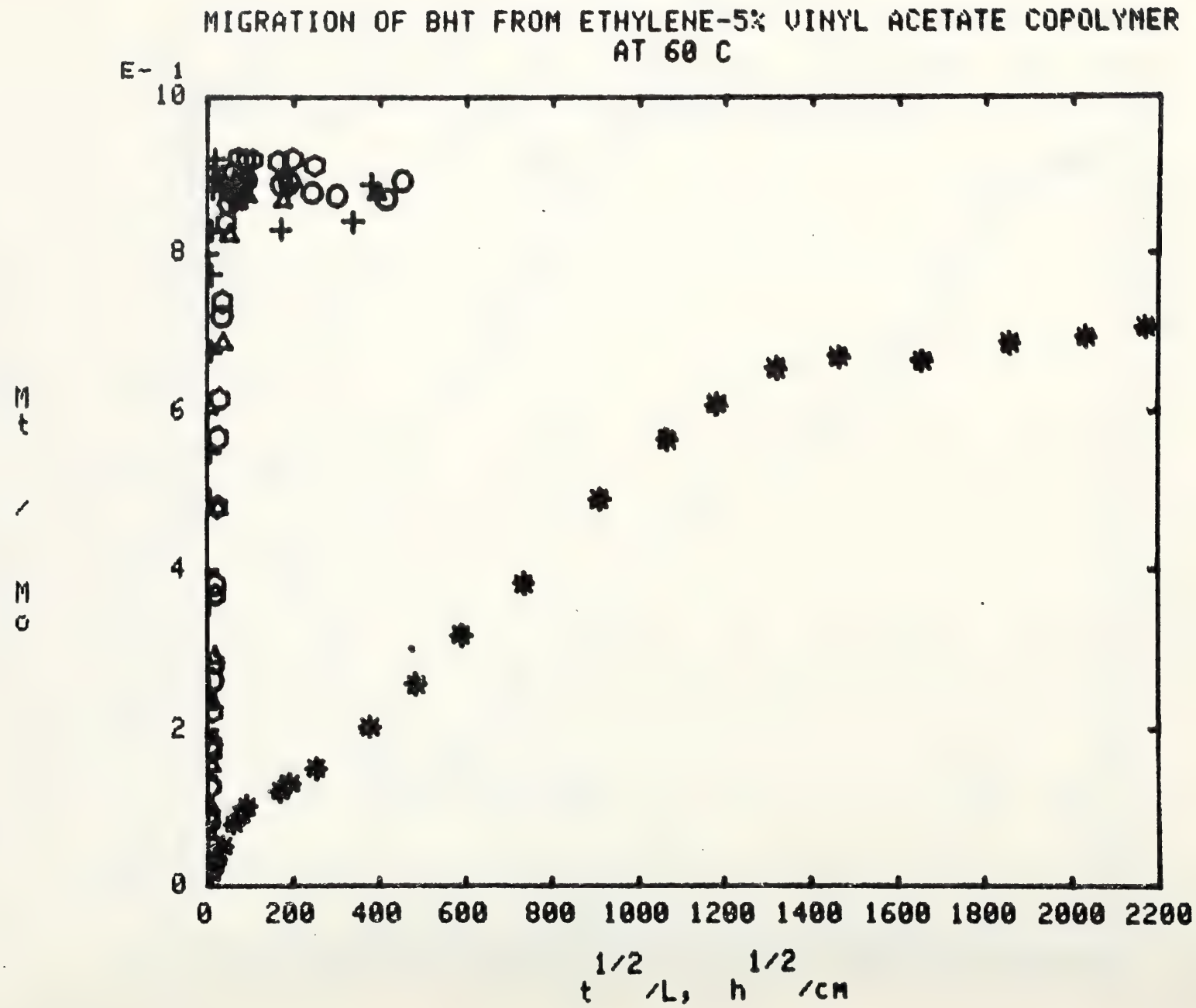

MIGRATION OF BHT FROM ETHYLENE-5% VINYL ACETATE COPOLYMER
AT 60 C
E- 1
10
8
6
4
2
0
M
t
/
M
o
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
t 1/2 /L, h 1/2 /cm

Figure V-1.3-A

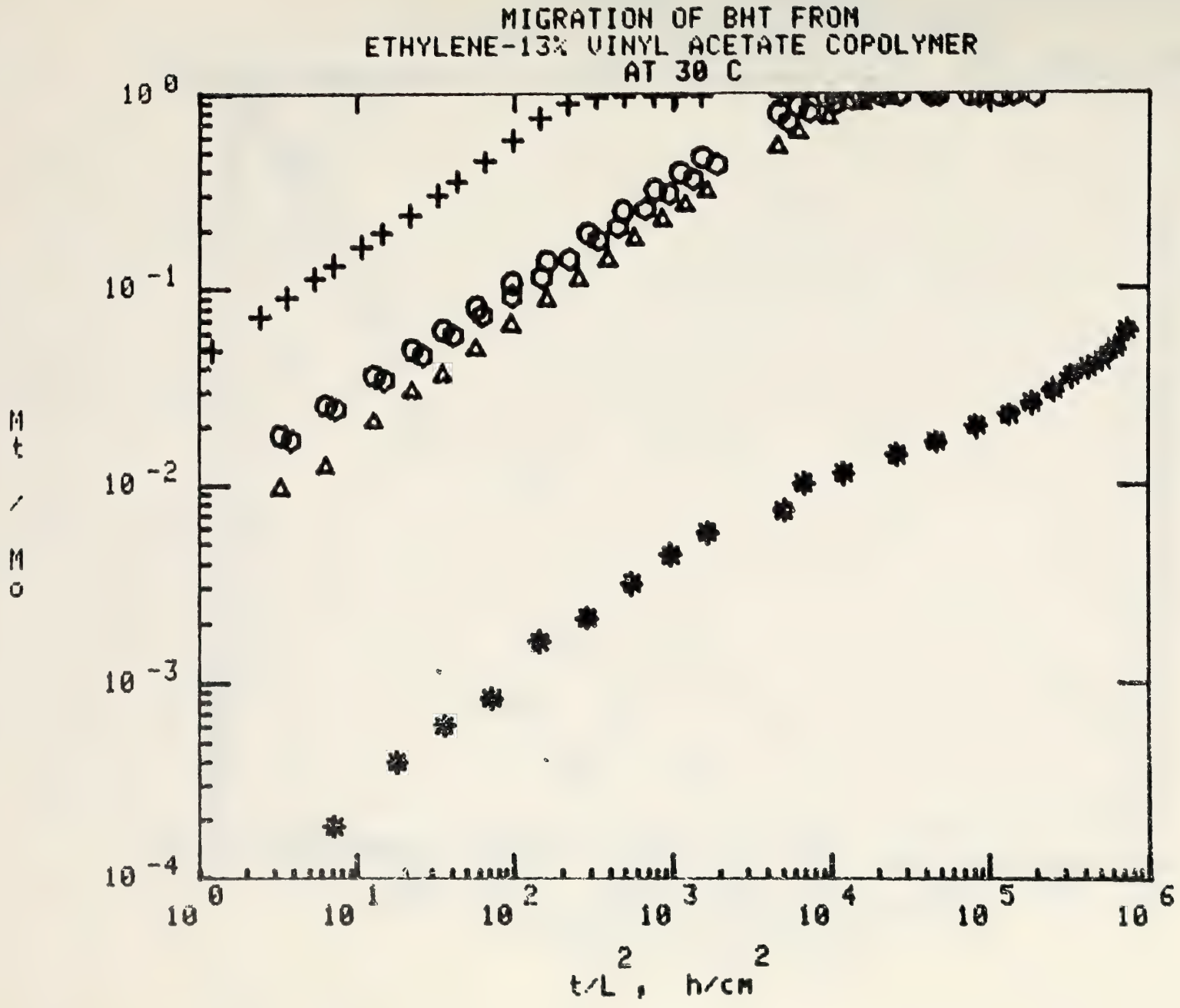

MIGRATION OF BHT FROM
ETHYLENE-13% VINYL ACETATE COPOLYMER
AT 30 C
10 0
10 -1
10 -2
10 -3
10 -4
M t / M o
10 0
10 1
10 2
10 3
10 4
10 5
10 6
t/L 2 , h/cm 2

Figure V-1.3-B

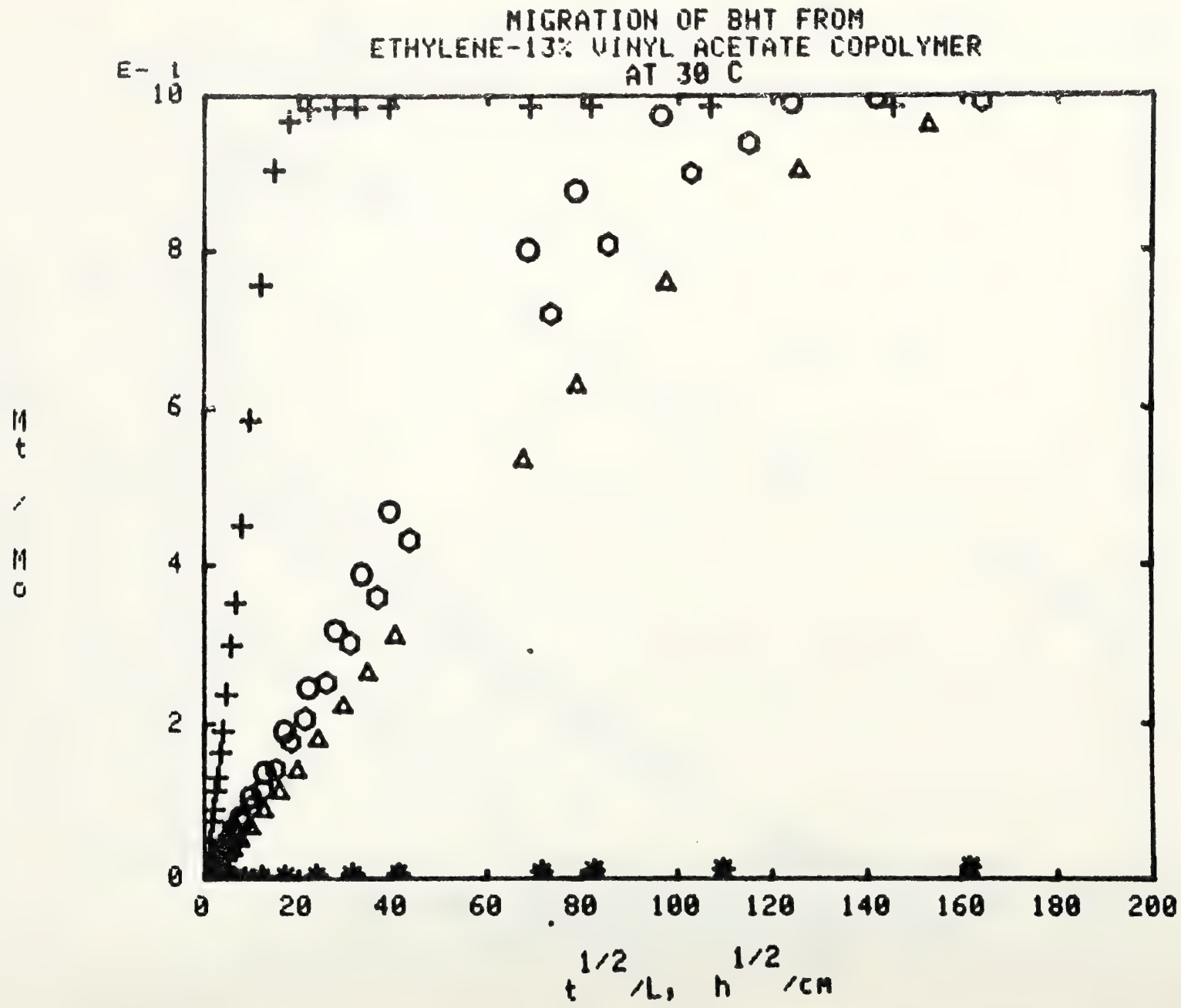

MIGRATION OF BHT FROM
ETHYLENE-13% VINYL ACETATE COPOLYMER
AT 30 C
E-1
10
8
6
4
2
0
Mt / Mo
0
20
40
60
80
100
120
140
160
180
200
t 1/2 /L, h 1/2 /cm

Figure V-1.3-C

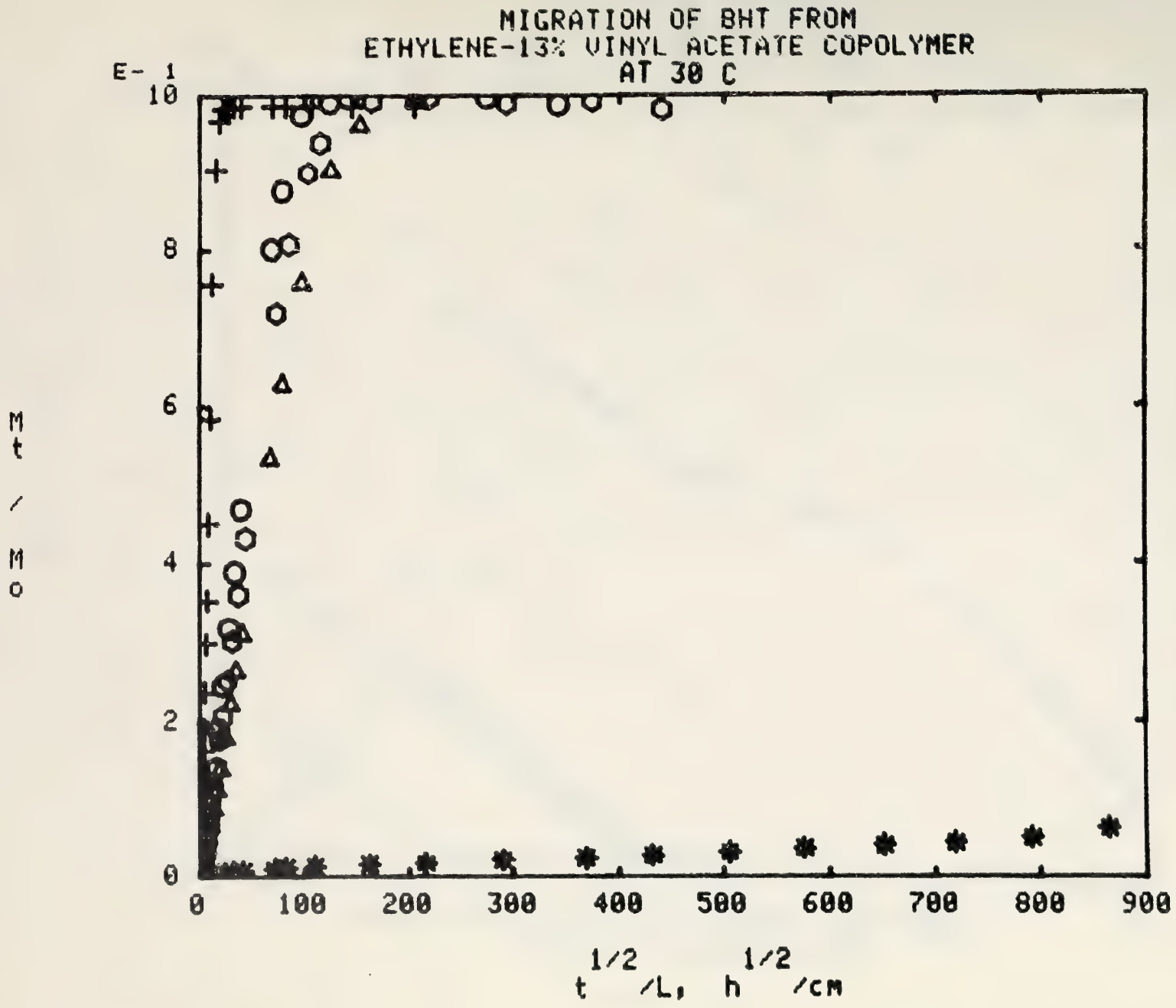

MIGRATION OF BHT FROM
ETHYLENE-13% VINYL ACETATE COPOLYMER
AT 30 C
E- 1
10
8
6
4
2
0
M
t
/
M
o
0
100
200
300
400
500
600
700
800
900
t 1/2 /L, h 1/2 /cm

Figure V-1.4-A

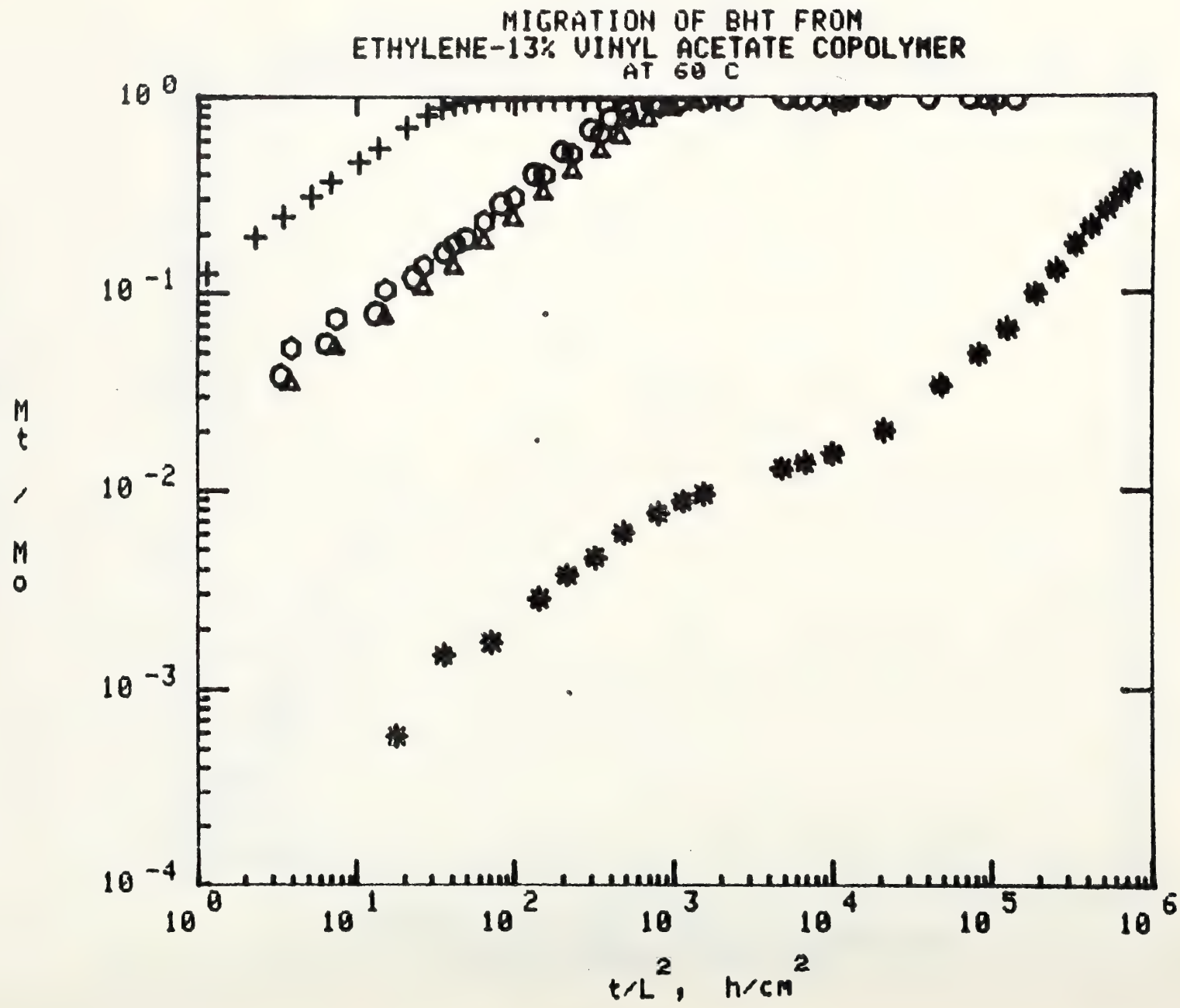

MIGRATION OF BHT FROM
ETHYLENE-13% VINYL ACETATE COPOLYMER
AT 60 C
Mt / Mo
10 0
10 -1
10 -2
10 -3
10 -4
10 0
10 1
10 2
10 3
10 4
10 5
10 6
t/L 2, h/cm 2

Figure V-1.4-B

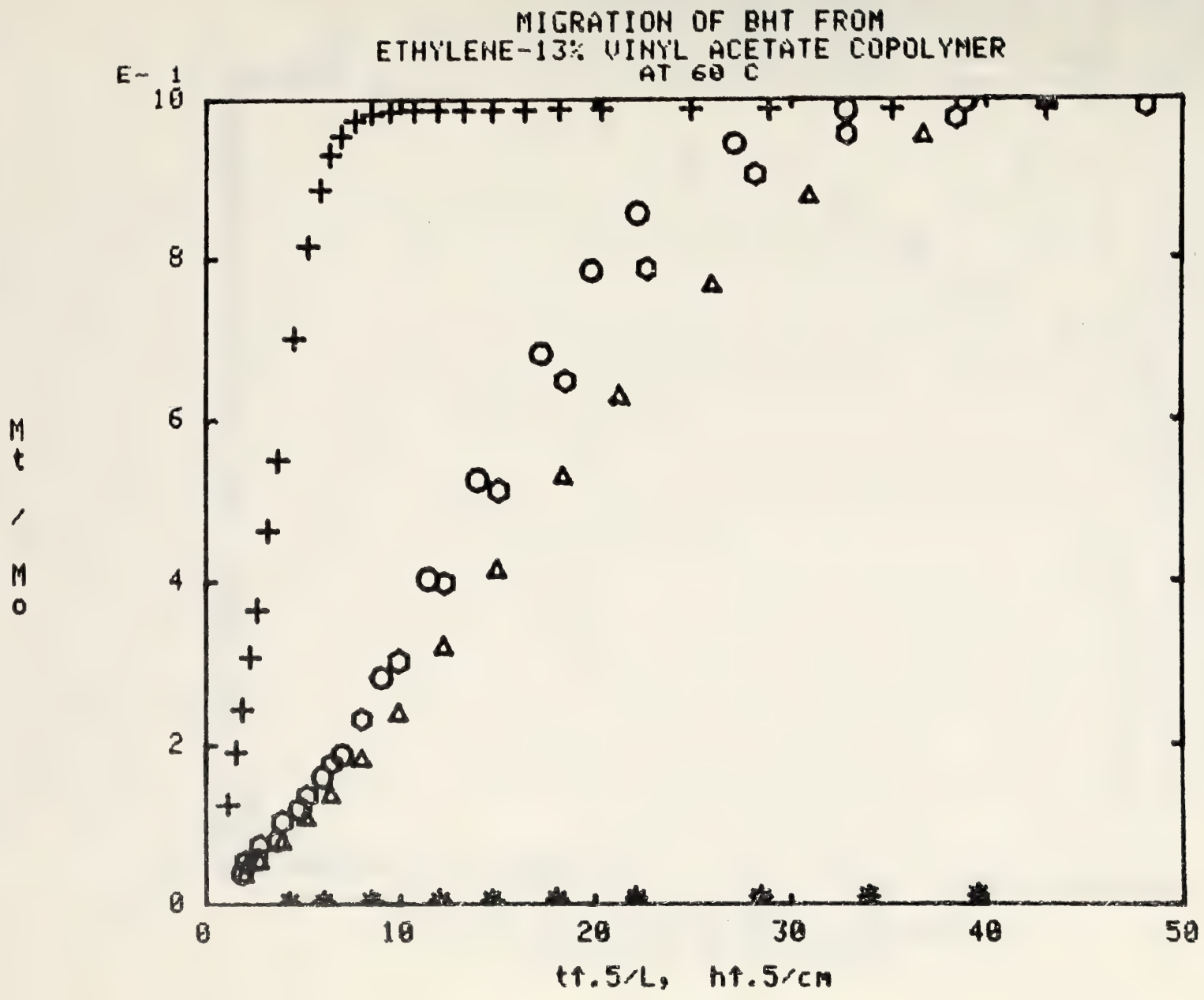

MIGRATION OF BHT FROM
ETHYLENE-13% VINYL ACETATE COPOLYMER
AT 60 C
E- 1
10
8
6
4
2
0
M
t
/
M
o
0
10
20
30
40
50
tt.5/L, ht.5/cm

Figure V-1.4-C

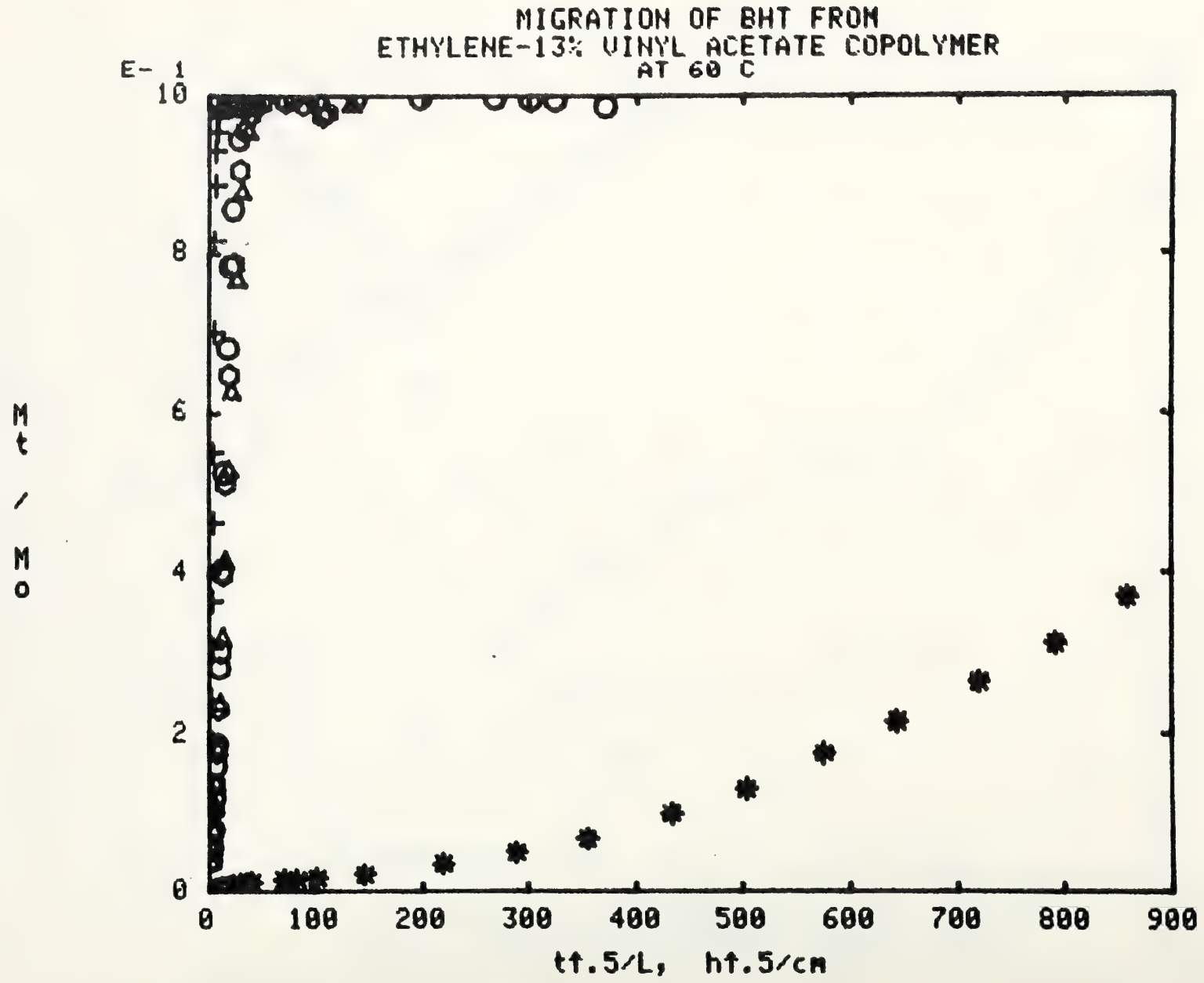

MIGRATION OF BHT FROM
ETHYLENE-13% VINYL ACETATE COPOLYMER
AT 60 C
E- 1
10
8
6
4
2
0
Mt / Mo
0
100
200
300
400
500
600
700
800
900
tt.5/L, ht.5/cm

Figure V-2.1 Migration of BHT from E-VA Copolymers into n-Heptane

Figure V-2.2 Migration of BHT from E-VA Copolymers into Corn Oil

Figure V-2.3 Migration of BHT from E-VA Copolymers into Ethanol

Figure V-2.4 Migration of BHT from E-VA Copolymers into 95% Ethanol

Legends for Figure V-2

	E-5% VA	E-13% VA
30°C	+	◇
60°C	x	□

Figure V-2.1

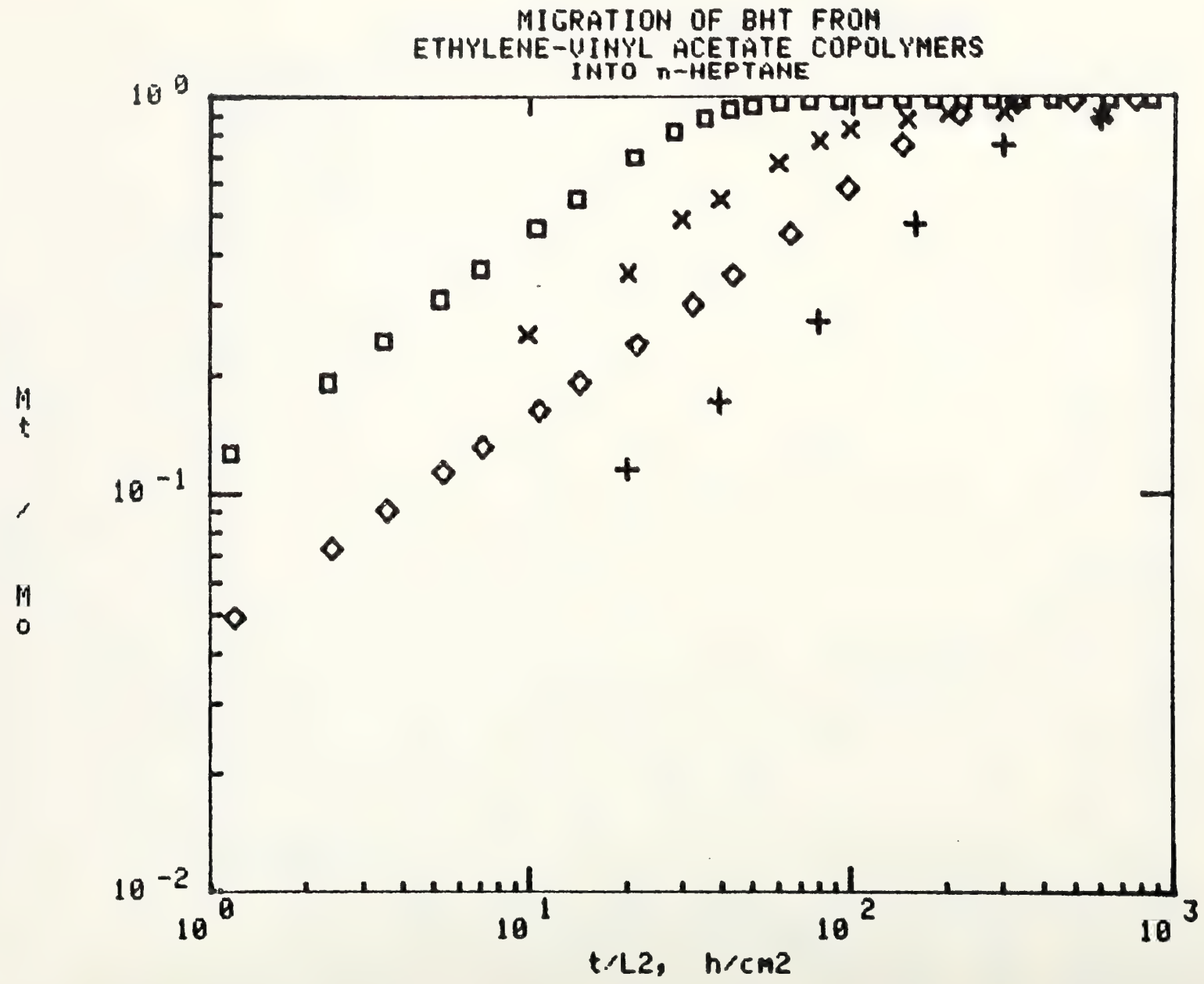

MIGRATION OF BHT FROM
ETHYLENE-VINYL ACETATE COPOLYMERS
INTO n-HEPTANE
10 0
10 -1
10 -2
M
t
/
M
o
10 0
10 1
10 2
10 3
t/L2, h/cm2

Figure V-2.2

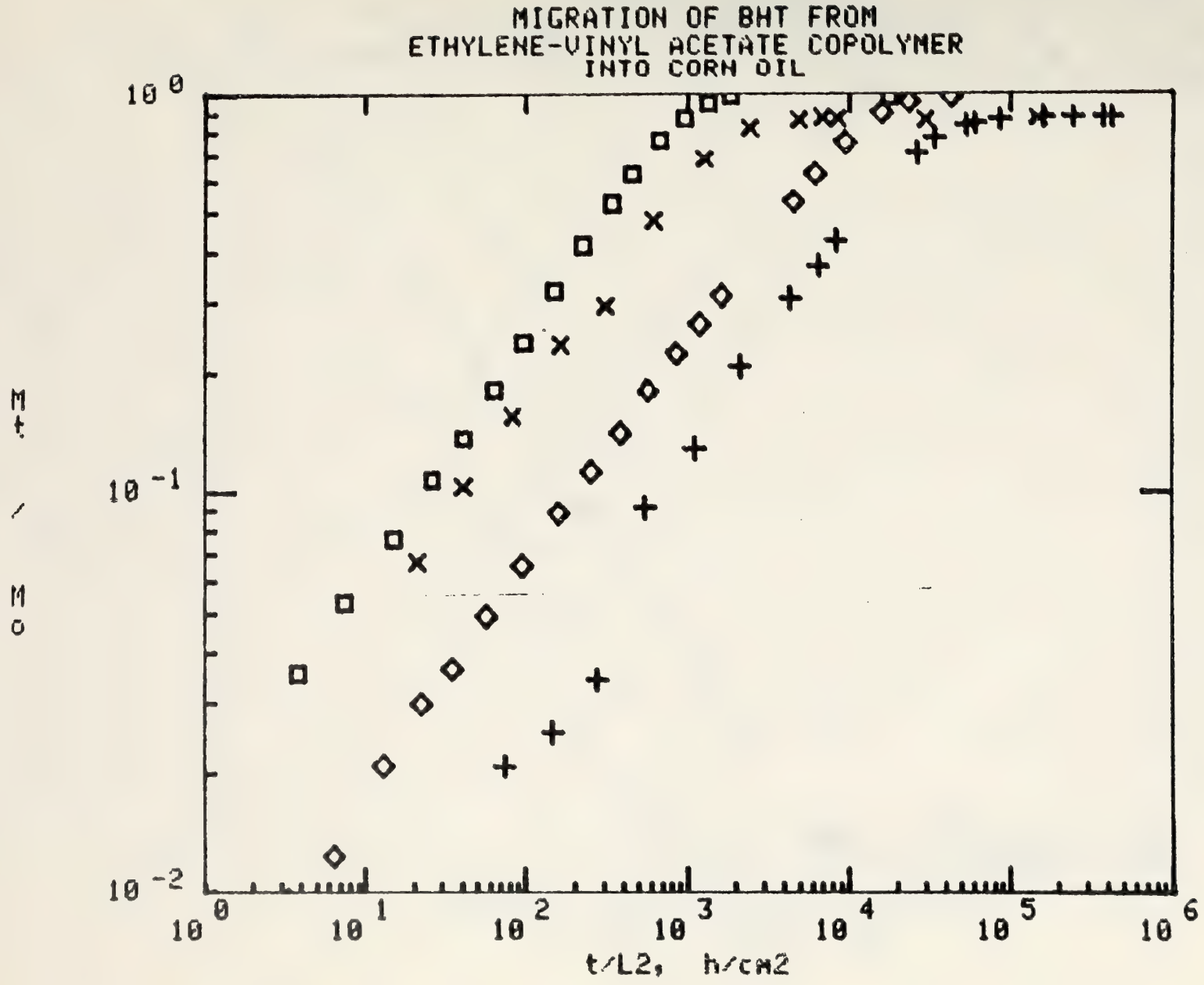

MIGRATION OF BHT FROM
ETHYLENE-VINYL ACETATE COPOLYMER
INTO CORN OIL
10 0
10 -1
10 -2
M t / M o
10 0
10 1
10 2
10 3
10 4
10 5
10 6
t/L2, h/cm2

Figure V-2.3

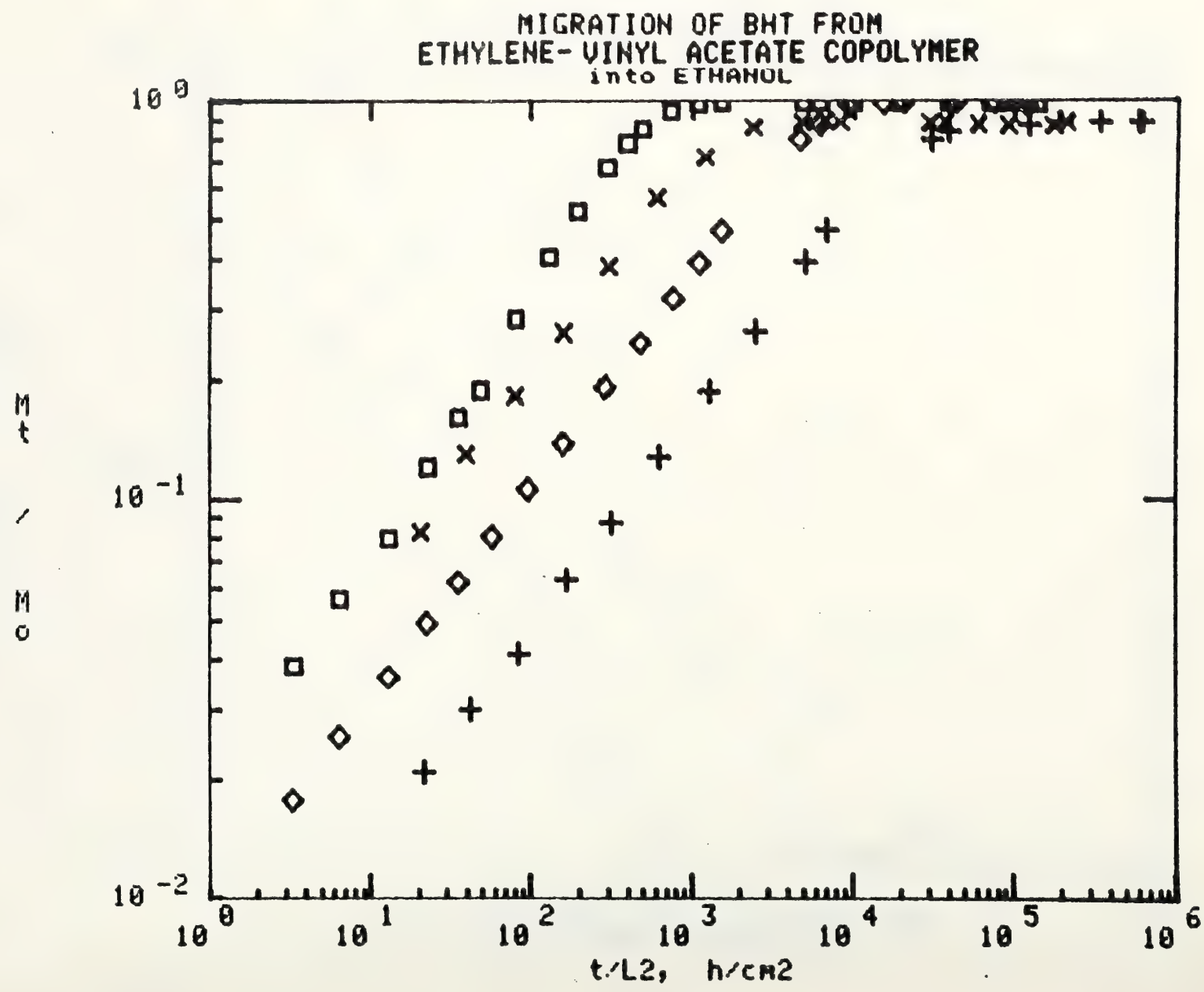

MIGRATION OF BHT FROM
ETHYLENE-VINYL ACETATE COPOLYMER
into ETHANOL
10 0
10 -1
10 -2
M t / M o
10 0
10 1
10 2
10 3
10 4
10 5
10 6
t/L2, h/cm2

Figure V-2.4

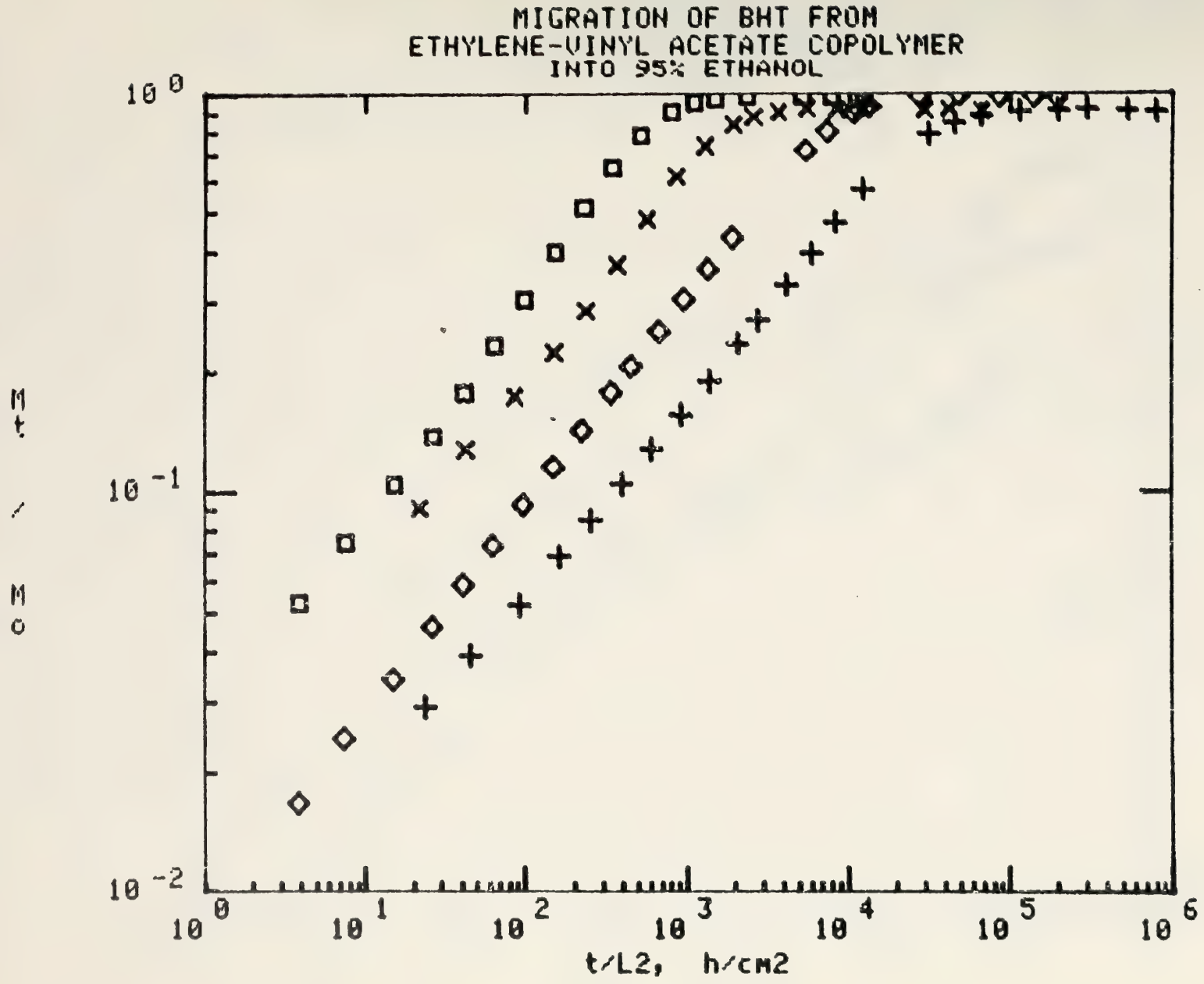

MIGRATION OF BHT FROM
ETHYLENE-VINYL ACETATE COPOLYMER
INTO 95% ETHANOL
10 0
10 -1
10 -2
M t / M o
10 0
10 1
10 2
10 3
10 4
10 5
10 6
t/L2, h/cm2

Figure V-3 A, B, C Migration of BHT from E-VA Copolymers into Water

Legends

	E-5% VA	E-13% VA
30°C	+	◇
60°C	x	□

Figure V-3-A

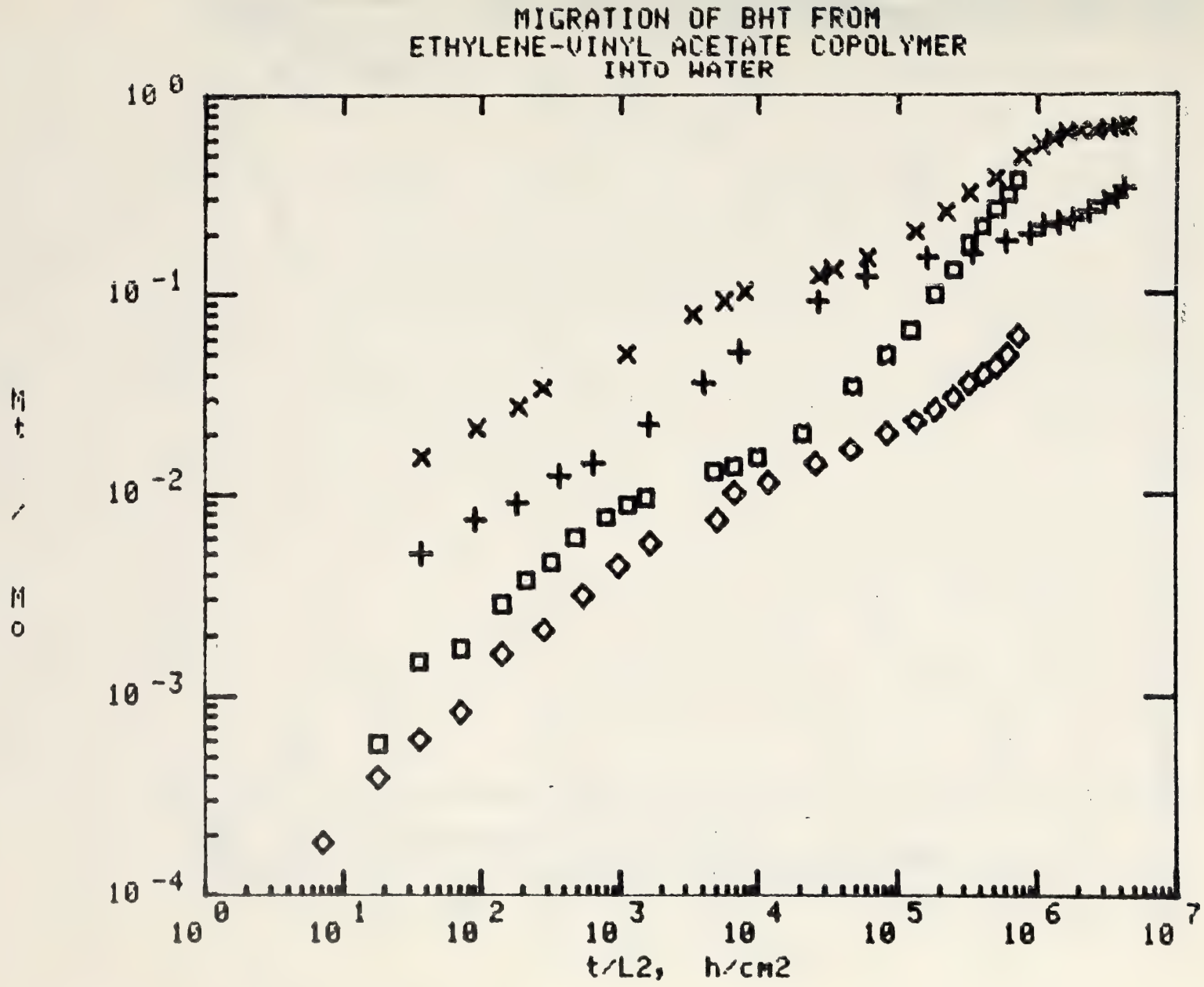

MIGRATION OF BHT FROM
ETHYLENE-VINYL ACETATE COPOLYMER
INTO WATER
10 0
10 -1
10 -2
10 -3
10 -4
Mt / Mo
10 0
10 1
10 2
10 3
10 4
10 5
10 6
10 7
t/L2, h/cm2

Figure V-3-B

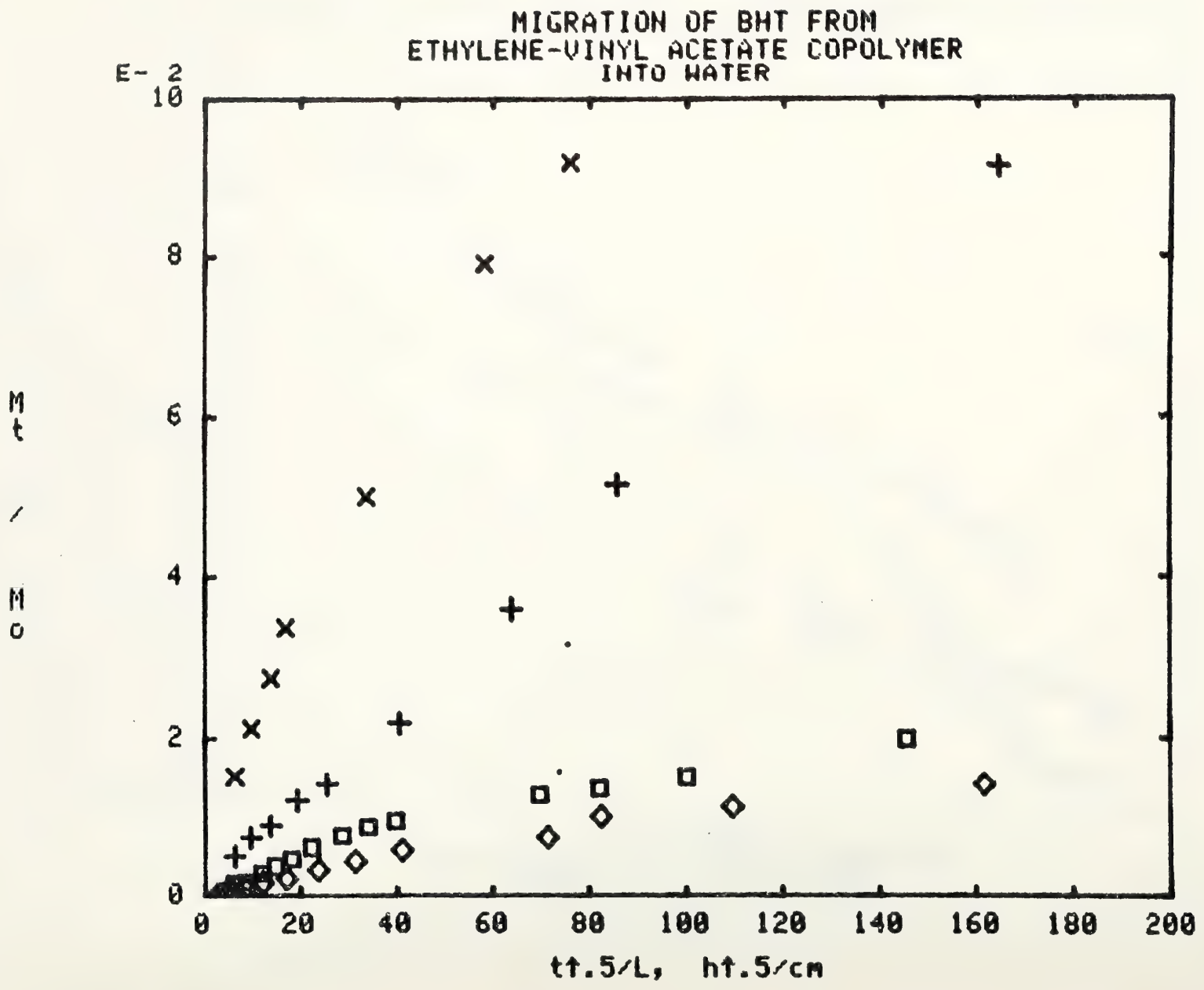
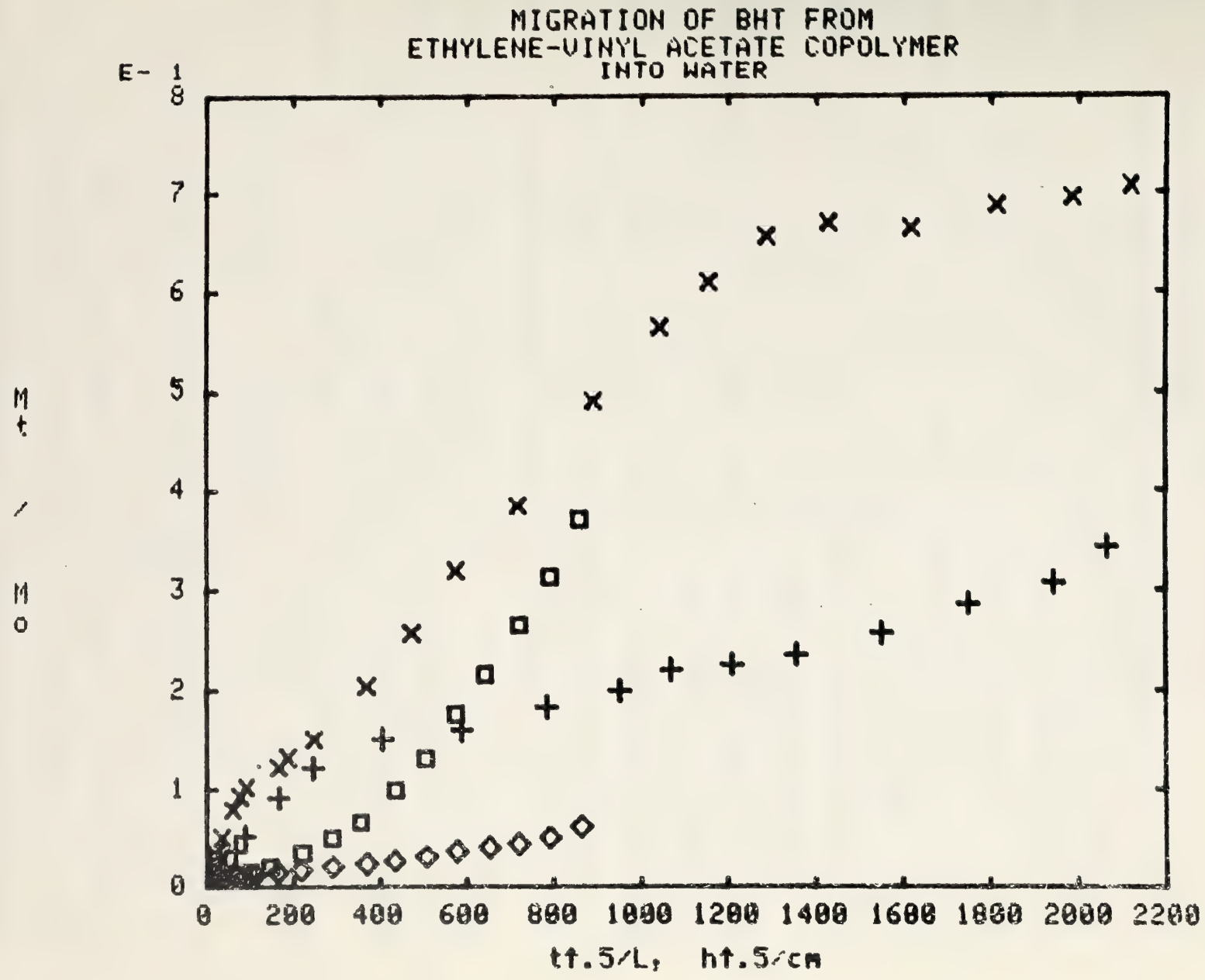

MIGRATION OF BHT FROM
ETHYLENE-VINYL ACETATE COPOLYMER
INTO WATER
E- 2
10
8
6
4
2
0
Mt / Mo
0
20
40
60
80
100
120
140
160
180
200
tt.5/L, ht.5/cm

Figure V-3-C


MIGRATION OF BHT FROM
ETHYLENE-VINYL ACETATE COPOLYMER
INTO WATER
E- 1
8
7
6
5
4
3
2
1
0
M
t
/
M
o
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
tt.5/L, ht.5/cm

VI. IGC Determinations of the Relative Diffusion Coefficients of Several Probes in Linear Polyethylene

Inverse gas chromatography (IGC) studies on the determination of diffusion constants in polyethylene were reported in the previous annual report [1]. These findings indicate that while accurate absolute diffusivity measurements seem beyond the reach of the IGC method, the possibility exists for using the technique to rank the relative ease of diffusion of many probes in a given polymer. A calibration of a specific column can be accomplished by conducting experiments with a probe-polymer combination of known diffusivity to calculate the mean polymer layer thickness from the measured peak broadening. The same column can then be used under similar operating conditions to determine other probe diffusivities and a relative ranking of many probe diffusion coefficients can be established. Experiments on several series of compounds have been conducted and those for which the data analysis and reduction have been completed will be used to illustrate the procedure of relative diffusivity determinations. Preceding this discussion, however, will be: a review of the theory for determining absolute diffusion constants from IGC studies, a summary of results from polyethylene-octadecane experiments to be used in the relative diffusivity determinations, and a section giving experimental details on the relative diffusivity measurements.

A Review of Pertinent Theory for IGC Absolute Diffusivity Determinations

The probe or migrant injected onto a chromatographic column resides partly in the carrier gas and partially in the polymer or stationary phase during transit through the column. Diffusion of the probe vapor in the gas phase can occur parallel to the background flow of carrier gas sweeping the vapor through the column both in the direction of and opposed to the carrier flow. This longitudinal or axial gaseous diffusion process causes an increase

in width of the eluted peak over its initial injection distribution. An additional gas phase peak spreading mechanism originates in the multiplicity of path lengths possible around the packed support particles and leads to an associated broadened distribution of elution times. Peak spreading can also be attributed to diffusive processes in the stationary phase. If the carrier gas flow rate is very rapid, steady-state partitioning of the vapor between the gas and stationary phases cannot be established. The residence time in the stationary polymer phase is then influenced by both the diffusivity of the probe in the polymer and the distance in the stationary phase over which diffusion must occur, among other factors. The peak broadening processes discussed above are commonly quantified by the convenient construct of the height equivalent to a theoretical plate, H, which is related to the width at half-height, $w_{1/2}$, for an eluted Gaussian-shaped peak as follows:

$$H = \frac{L}{8 \ln(2)} \left(\frac{w_{1/2}}{t_R} \right)^2 \qquad (1)$$

where L is the column length, and t_R the retention time of the peak at the maximum. The determination of these quantities from a Gaussian-shaped experimental chromatogram with a peak standard deviation of σ is illustrated in the schematic of Figure VI-1.

An equation attributed to van Deemter et al. [2] is often used to relate H to the local carrier gas flow velocity, u, and is of the form:

$$H = A + B/u + Cu \qquad (2)$$

The A term arises from the number of possible gas paths through the column; B is from longitudinal diffusion of the probe in the carrier gas; and C originates from the resistance to mass transfer in the polymer or stationary

phase. The coefficients in equation 2 are defined as follows:

$$A = 4\lambda r \tag{3}$$

$$B = 2\gamma D_g \tag{4}$$

$$C = \frac{8\ s^2 k}{\pi^2\ D_s (1 + k)^2} \tag{5}$$

where λ is a measure of support packing irregularities, r the average support particle radius, γ a correction coefficient for constriction and tortuosity of the gas flow path in the column, D_g the probe diffusivity in the gas phase, s the effective thickness of the stationary phase film, D_s the diffusivity of the probe in the stationary phase, and k the column capacity factor commonly given as:

$$k = \frac{t_R - t_M}{t_M} \tag{6}$$

where t_M is the time taken to elute an unsorbed marker material from the column. Equation 2 indicates that, at large values of the flow rate, H will be proportional to the flow rate. The probe-polymer diffusion coefficient can then be determined from the constant of proportionality C by equation 5 if the effective film thickness is known. Equation 5 is not applicable for columns packed with glass bead support particles. In such cases of diffusion into a uniform stationary phase film on a solid surface, a similar relation for C applies:

$$C = \frac{2\ s^2 k}{3\ D_s (1 + k)^2} \tag{7}$$

While equation 2 gives a suitable explanation of peak spreading in some cases, other results have raised questions about its utility, particularly when significant gas phase diffusion can occur. These discrepancies indicate that the simplifications made by van Deemter in neglecting other mechanisms of diffusion are not valid for all systems. Giddings and coworkers [3] examined several modified forms of the van Deemter equation and found that none could account for the experimental results obtained on columns of varying length and outlet pressure.

An equation proposed by Jones [4] takes several additional sources of peak spreading into consideration: resistance to mass transfer in the gas phase normal to the carrier gas flow direction (D), carrier gas velocity distribution effects (E), and a correlation between these two processes (F). This equation is given as:

$$H = A + B/u + (C + D + E + F)u \tag{8}$$

where C is as in equation 7 and

$$D = \frac{C_D\, k^2\, g^2}{D_g(1 + k)^2} \tag{9}$$

$$E = \frac{4C_E\, r^2}{D_g} \tag{10}$$

$$F = \frac{4\theta(C_D C_E)^{1/2}\, k\, r\, g}{D_g(1 + k)} \tag{11}$$

g being the diffusion path length in the gas, θ the correlation coefficient between the D and E terms, and C_D and C_E geometric constants.

The radial diffusion D term was discounted by van Deemter and co-workers in the derivation of equation 2 because of the much greater magnitude of D_g compared to D_s. This simplification is valid for the thick liquid films used in their work, studies of columns with roughly 0.3 mass fraction stationary phase loading. The diffusion distances s and g are roughly comparable under these circumstances. If low column loadings which reduce s to about 0.01g are used, then the much larger probe diffusivity in the gas phase is overcome by the ease of mass transfer through the thinly-spread liquid phase and the D term cannot be ignored.

The E contribution to spreading arises from diffusion caused by differences in the velocity of the carrier gas in various parts of the column. Velocity differences can arise from both short and longer range channels formed by support packing irregularities and from trans-column effects caused by the influence of the tube walls. These effects are summarized by Giddings [5] who estimates approximate magnitudes for contributions of the many possible velocity gradients combined in the E term of equation 8.

While the first three terms in equation 8 are independent of one another, the D and E terms are not since molecules which have a lower average velocity will spend a smaller fraction of time in the gas phase and therefore not experience as great a percentage of gaseous diffusion as molecules with higher than average velocity. The total variance, σ_{ij}^2, of two such dependent contributors, σ_i^2 and σ_j^2, is given as:

$$\sigma_{ij}^2 = \sigma_i^2 + \sigma_j^2 + 2\theta_{ij}\sigma_i\sigma_j \qquad (12)$$

where the correlation coefficient between the two contributors is denoted as θ. The F term of equation 11 originates from the final term in the above relation and corresponds to the interaction between the D and E terms.

Giddings [6] has given an expression said to account for all known plate height terms contributing at least one percent of the total plate height for packed GC columns in the absence of interfacial adsorption as:

$$H = \sum_i \frac{1}{1/A_i + 1/E_i u} + \frac{B}{u} + \sum_i C_i u + Du + G \qquad (13)$$

The G term represents the contribution of column-wide velocity inequality effects, such as that arising from column coiling, and could alternatively be included in E. This equation is otherwise similar to equation 8 except for its omission of the interaction term F. A compilation of the C, D, and E coefficients expected to apply in various situations and a means of calculating their magnitude from measurable column parameters is given in reference [5].

The plate height equations discussed up to this point apply only to the peak spreading in a short region of the chromatographic column where the carrier velocity u is a constant local to that region. A final modification can be made to equation 8 or 13 to account for the variation in local carrier velocity along the column caused by the drop in pressure from column inlet to outlet. The effect of this correction is primarily on the liquid mass transfer term, as discussed by Dal Nogare and Juvet [7]. The final expression for the dependence of the experimentally accessible column average plate height, $\bar{H}$, on the carrier gas outlet velocity, u_o, is similar to equation 8 and is given as:

$$\bar{H} = A + \frac{B}{u_o} + \left(\frac{2p_o C}{p_i + p_o} + D + E + F + G \right) u_o \qquad (14)$$

where p_i and p_o are the column inlet and outlet pressure. The gas phase diffusivity found in equations 4, 9, 10, and 11 must also be restated at the outlet pressure of the column. The form of this modification is based on the relationship between the local column velocity and the average carrier gas velocity. The preceeding treatment assumes a distance average of this velocity. Other methods [3] involve the use of a pressure average velocity and yield a slightly different equation for $\bar{H}$ but agree reasonably well with equation 14 even at large values of the inlet pressure.

The magnitudes of coefficients in equation 14 and the configuration of the polymer film on the surface of the supporting beads can have a significant influence on the methods used in interpreting data derived from IGC determinations of diffusive peak broadening as discussed in the previous annual report. These effects will be reviewed briefly for the experimental determination of the diffusivity of normal octadecane in high density polyethylene considered there.

Summary of Previous Results for LPE-Octadecane

As discussed earlier, IGC determinations of diffusivity in the polymer phase are made from a study of probe peak broadening at varying carrier gas velocities; a schematic illustration of the results is shown in Figure VI-2. The local plate height and carrier velocity of equation 2 are commonly replaced by the measured average quantities in experimental determinations of column efficiency. Such $\bar{H}$ vs $\bar{u}$ plots for eight flow velocities in the flow rate region from about 10 to 100 cm/s yielded a slope C for column A of 7.05 ms with calculated standard deviation of 8.8 percent and 18.9 ms with calculated standard deviation of 7.4 percent for B. The van Deemter treatment provides for the calculation of the diffusivity of C_{18} in linear

polyethylene from these C values by equation 7 when the polymer film thickness in each column is known. Such a procedure is proper only if the other contributions to peak spreading discussed earlier are small when compared to that arising from polymer or stationary phase mass transfer. This assumption has been made in many previous studies of probe-polymer diffusion. However, if the other gas phase kinetic processes are operating to a significant extent then the limiting slope at high flow rate of Figure VI-1 should also reflect these contributions, as indicated by equations 8 and 14. It was important, therefore, to estimate the relative magnitude of the gas phase terms as compared to the stationary phase contribution to determine if such a simplified data analysis procedure could be applicable.

A further consideration is the nature of the carrier velocity on which the plate height depends. Equation 14 indicates that while the plate height contribution of the B, D, E, and F terms are directly or inversely proportional to the carrier outlet velocity u_o, the C term contribution to $\bar{H}$ depends on the average velocity. Consequently, the often-employed plot of $\bar{H}$ vs average carrier velocity suggested by equation 2 will not be linear at high flow velocity for any variant of velocity if both stationary and gas phase mass transfer effects are nonnegligible.

The estimated gas phase contributions to peak spreading were computed for both columns and compared to the limiting slope C calculated from the van Deemter equation least squares fit. It was evident that the peak spreading attributed to gas phase diffusion made a significant contribution to the overall kinetic broadening for column A. In instances of this nature, where gas phase diffusion terms make a significant contribution to peak spreading, difficulty can be encountered in deciding which are important and calculating their values. Alternatively, it is possible to resolve the gas and stationary

phase mass transfer contributions without directly estimating the magnitude of the gas phase terms. Purnell [8] has suggested a method which involves first determining A and B of equation 14 and employing these values to reduce the experimental $\bar{H}$ to the peak spreading arising only from mass transfer effects, $\bar{H}'$. In terms of an equation:

$$\bar{H}'/u_o = \left(\bar{H} - A - \frac{B}{u_o} \right) \Big/ u_o = \frac{2p_o}{p_i + p_o} C + D + E + F + G \qquad (15)$$

When the left-hand side of this equation is plotted against the pressure correction $2p_o/(p_i + p_o)$, a straight line with slope C and intercept (D + E + F + G) should be obtained. Evaluation of the constants A and B requires that experiments be conducted over a wide range of carrier gas flow velocities. Limited low velocity data often precludes experimental determination of these constants in many cases; however, they can be estimated from theoretical considerations and experimental results. The multipath A term defined in equation 3 has been determined to have a λ value between one half and unity in many cases [9] and a value of 0.5 was assumed here. The longitudinal diffusion B term most often has a γ value near one [9] and unity was utilized in the determinations. These values were used to calculate the A and B terms of equation 19 and a fit of $\bar{H}'/u_o$ against the pressure correction term gave a linear least squares line with a slope of 16.4 ms and calculated standard deviation of 5.5 percent for column A and 21.9 ms with calculated standard deviation of 6.6 percent for B. These results are compared to the van Deemter fit slopes in Table VI-1 on the following page. The smaller standard deviations of the Purnell method slopes compared to the corresponding values for the van Deemter fit discussed earlier indicated the better applicability of the Purnell method. The C value obtained by this method for column A was more

Table VI-1

Comparison of the C Coefficient Determined by Two Methods for LPE-Octadecane at 150 °C

Column Code	Column Loading (Mass Fraction Polymer)	$C_{van\ Deemter}$ (Eq. 2)	$C_{Purnell}$ (Eq. 15)
A	6.10×10^{-4}	7.05 ms	16.4 ms
B	5.71×10^{-3}	18.9 ms	21.9 ms

than twice that obtained from the van Deemter analysis. This was attributed to the latter's combination of the effects of polymer and gas phase mass transfer in a nonlinear manner, which can be noted by comparing the C term appearing in equation 2 to its complement in equation 14, the expression in parenthesis. For the case of column A where the gas phase terms contributed significantly to the peak broadening, the van Deemter equation-based analysis underestimated the magnitude of C. Gas phase mass transfer effects for column B contributed only slightly to the total broadening and this was reflected in the similar results of the two methods for determining C which differed by only 15 percent, as indicated in Table VI-1.

While the method of determining the polymer phase mass transfer contribution can be important under certain column conditions, the most significant parameter which affected the diffusivity determination was the distance over which diffusion occurred. This distance is commonly identified with the effective film thickness s of equation 7. It is often assumed that the stationary phase is distributed as a uniform thin film over the entire surface of the spherical glass bead column packing. The effective film thickness for this geometry can be calculated from the expression:

$$s = \frac{M_s}{4\pi r^2 N \rho_s} \qquad (16)$$

where M_s is the mass of polymer phase in the column, N the number of support particles in the column, and ρ_s the polymer density. Such a configuration requires a high amount of stationary phase surface area, however, and a geometry in which the stationary phase is confined by capillary forces into annular regions around the contact points between support particle spheres has been advocated as a means of minimizing the exposed stationary phase surface area. This geometry has been observed for both low molecular weight [6] and polymeric [10] stationary phases coated onto glass bead supports and is illustrated schematically in Figure VI-3. A stationary phase film may also be present on surfaces where the beads are not in contact, as indicated in the inset. Its thickness, however, should be much less than that of the stationary phase in the region of adjacent support beads.

The different diffusion path lengths expected for the two extremely different polymer distributions described above can exert a significant influence on determinations of polymer-probe diffusivity by IGC. Giddings [11] has compared the contribution to peak spreading expected from a hypothetical support coated with two regions, a thin film of uniformly adsorbed stationary phase and a second region where the liquid stationary phase collects at the support contact points. He concludes that for glass bead supports at mass fraction loadings up to about 0.015, the bulk of the stationary phase is present at the bead contact points and controls the plate height performance by virtue of its greater thickness. An equation has been proposed [12] to relate C to measurable column parameters for this geometry and is as follows:

$$C = \frac{r^2 k}{3\, D_s (1 + k)^2} \left(\frac{m_s \rho}{18.75 \rho_s} \right)^{1/2} \qquad (17)$$

where ρ is the density of the support particles and m_s the mass fraction of polymer phase in the column. This treatment assumes that the spherical support particles pack randomly and are surrounded by 6.25 nearest neighbors. The relation for C is similar in form to equation 7. If the differing variables are combined into an explicit expression for s in terms of the particle size, the following relation is obtained:

$$s = \left(\frac{m_s \rho}{18.75 \rho_s} \right)^{1/4} \frac{r}{2\sqrt{5}} \qquad (18)$$

This equation provides for the calculation of a value of s which, when substituted into equation 7, yields a result for C identical to the C term determined by equation 17.

A computation of s by these methods was useful for comparing the effective film thicknesses of the two stationary phase arrangements considered. The average film thicknesses calculated in the above manner for a polymer stationary phase collected at bead contact points were much greater than the thicknesses corresponding to the uniform layer geometry, as can be noted from the following table.

Table VI-2

Effective Layer Thicknesses for Columns with Differing Polymer Phase Geometry

Column Code	Effective Layer Thickness, s(μm)	
	Uniform Thin Surface Film (Eq. 16)	Annular Film at Contact Points (Eq. 18)
A	0.043	5.58
B	0.404	9.77

Both equations 7 and 17 were used to calcualte the diffusion coefficient of octadecane in HDPE. For column A assuming a thin uniform film, D_s was calculated from the C coefficient obtained with the Purnell treatment by substituting equation 16 into equation 7; a result of 3.8×10^{-11} cm^2/s was obtained. Assuming a geometry where the polymer collects at the bead contact points for column A, D_s was calculated according to equation 17 and a value of 6.4×10^{-7} cm^2/s determined. These results and the corresponding values for column B are summarized in Table VI-3 below.

Table VI-3

Influence of Film Geometry on the Diffusion Coefficient of Octadecane in Linear Polyethylene at 150 °C

Column Code	Diffusion Coefficient ($cm^2 \cdot s^{-1}$) Uniform Thin Surface Film (Eqs. 7 and 16)	Annular Film at Contact Points (Eq. 17)
A	3.8×10^{-11}	6.4×10^{-7}
B	4.1×10^{-10}	2.4×10^{-7}

It was evident that the uniform thin film geometry assumption led to unreasonably low values of the diffusion coefficient. In addition, an order of magnitude discrepancy existed between results for the two columns. The assumption of a collection of the polymer stationary phase at bead contact points yielded diffusion coefficients of reasonable magnitude for the temperature of the experiment and column-to-column agreement within a factor of three. This threefold difference in the diffusivity results may be attributed to the effects of differing probe concentrations in the polymer phase of the two columns.

Diffusivity values are often quite sensitive to the concentration of the diffusing species, depending approximately either linearly or exponentially

on concentration [13]. In these IGC determinations the probe concentration in the polymer film varied both along the column length due to increasing peak broadening with transit time and with the depth of penetration into the polymer film expected from Fickean diffusion. The diffusivity determined was therefore a concentration-averaged value over all column conditions. The actual concentration of octadecane in the polyethylene film was estimated to range from 0.01 to 1.5 percent by mass for column A and from 0.001 to 0.16 percent by mass for column B. The diffusion coefficient calculated from the column B results corresponded to probe concentrations about an order of magnitude lower than for column A. This could account for the lower value of probe diffusivity determined with column B. For either a linear or exponential dependence of the diffusion coefficient on concentration, the diffusivity should be less at lower diffusant concentrations, as found here. A determination of the functional relationship of the diffusivity on diffusant concentration was not possible, however, because of the variation in probe concentration along the column length and the limited amount of data available.

Limited data are available in the literature on diffusion of the higher alkanes in LPE; however, studies of similar diffusants, linear aliphatic esters with 25 to 45 backbone units, have been conducted by Klein and Briscoe [14]. Extrapolating their experimental results to an 18 unit chain leads to an expected diffusion coefficient of 5×10^{-6} cm^2/s in linear polyethylene at 152 °C. This result is about an order of magnitude greater than the IGC determinations for a polymer film collected at the support bead contact points.

The distribution of film thickness also plays an important role in determining the magnitude of the diffusivity. The previous calculations

assumed that the film thickness was constant. In an actual column, however, the film thickness would be expected to be distributed about the mean values employed here. An alternate form of equation 7 can be used to estimate the effects of different film thicknesses [15]. The equation is:

$$D_s = \frac{k}{C(1 + k)^2} \sum_i q_i x_i s_i^2 \qquad (19)$$

where q_i is a configuration factor and x_i the volume fraction per unit column volume of stationary phase segments with thickness s_i. Assuming a uniform configuration factor and holding x_i constant gives:

$$D_s = \frac{kqx}{C(1 + k)^2} \sum_i s_i^2 = Z \sum_i s_i^2 \qquad (20)$$

which reduces to:

$$D_s = Zs^2 \qquad (21)$$

for a uniform film of thickness s. For a distribution with an equal volume of film 0.1s and 10s in thickness:

$$D_s' = Z\,[5(0.1s)^2 + 0.05(10s)^2] = 5.05\ Zs^2 \qquad (22)$$

This distribution, resulting from the same volume of stationary phase present in the uniform thickness case, leads to a diffusivity value five times larger than that corresponding to a uniformly distributed film. Table VI-4 summarizes the effects of different thickness distributions on the diffusion coefficient D_s' compared to that expected from a uniform film of thickness s, D_s. All the geometries considered require the same volume of stationary phase per unit column volume and have an average thickness of s. It is evident from these examples that thick sections of the polymer film

Table VI-4

Effect of Thickness Distribution on Diffusivity in the Polymer Phase

Thin Section Depth	Thick Section Depth	D_s'/D_s
0.50s	2s	1.25
0.25s	4s	2.13
0.10s	10s	5.05
0.02s	50s	25.01
0.01s	100s	50.01

can exert a disproportionate influence and lead to a considerable increase in the polymer-probe diffusion coefficient when compared to the value calculated for an IGC experiment with an assumed ideal polymer layer of uniform thickness. An experimentally difficult determination of the variability of the polymer film in the IGC column would be necessary in order to correct the calculated diffusivity values for the actual polymer layer nonuniformity.

Experimental Details

The column used throughout the relative diffusivity study was prepared from glass support beads coated with a layer of the linear polyethylene (LPE) NBS SRM 1475 and packed into a 6.35 mm outer diameter stainless steel tube, as described in the previous annual report [1]. After installation in the gas chromatograph, a final drying and column conditioning step was carried out by purging with dry, deoxygenated helium followed by heating to 150 °C for a 24-hour period. The column used is identical to column B in the previous annual report and contains 5.71×10^{-3} mass fraction of LPE. It was chosen because of the relatively small contribution which gas phase mass transfer made to the overall peak spreading when compared to column A of that report.

Several alkane probes and an antioxidant were employed as diffusants and are listed in the table below [16]. All were dissolved in hexane (Burdick and Jackson Labs.) to give solutions of about 0.02, 0.2, and 2.0 percent by mass.

Table VI-5

Probes Employed in an IGC Study of Relative Diffusivity in LPE

Probe	Code	Source
n-octadecane	C_{18}	Supelco
n-hexadecane	C_{16}	Aldrich Chemical
2-methylpentadecane	$2MeC_{15}$	Alfa Products
2,2,4,4,6,8,8-heptamethylnonane	$7MeC_9$	Aldrich Chemical
n-tridecane	C_{13}	American Petroleum Institute
1,3-di-tert-butyl-2-hydroxy-5-methylbenzene	BHT	Polysciences

Approximately 1 µl of each solution was injected into the flash vaporization injector of a gas chromatograph, maintained at 180 °C. The column oven was held at 150 °C ± 0.3 °C throughout. The eluted peaks were monitored with a flame ionization detector (FID) held at 190 °C, whose signal at 10^{-10} A/mV sensitivity was fed to an electronic integrator connected to a strip chart recorder and to a high acquisition speed recorder-plotter. The former setup was employed to time the peak maxima to within 0.01 min and for manual measurements of the chart width at half maximum at chart speeds up to 1 cm/s. Typical results are shown in Figure VI-4.

The rapid collection capabilities of the high speed recorder-plotter allowed the FID output to be sampled at 10 ms intervals, facilitating analysis

of the marker and solvent peaks. A typical trace is shown in Figure VI-5 for five repeated determinations. Data collection was triggered upon injection of the methane and hexane vapor sample and the time to the methane peak maximum, assumed to have k = 0, was employed to determine t_M of equation 6 and to calculate the column average linear flow velocity, $\bar{u}$, from the expression:

$$\bar{u} = L/t_M \tag{23}$$

The quantity of interest, the column outlet velocity, was then calculated from $\bar{u}$ as follows:

$$u_o = \frac{2\bar{u}}{3}\left[\frac{(p_i/p_o)^3 - 1}{(p_i/p_o)^2 - 1}\right]. \tag{24}$$

Column inlet and outlet pressures were monitored with calibrated pressure gauges of appropriate range. The outlet pressure was very near to atmospheric in all cases. The helium carrier gas volumetric flow rate was measured with a soap film flow meter, when necessary. The data were collected over a corrected flow rate range of about 1 to 5 ml/s.

The first derivative of a chromatographic peak with respect to time can be used to aid in determinations of the maximum height and peak widths indicated in Figure VI-1. At a point where the chromatogram is at a maximum, the first derivative will be zero while the second derivative is negative. Determination of the first derivative zero point is illustrated with curve B of Figure VI-6, the first derivative of curve A obtained by experiment. The inflection points of the chromatogram are also readily indicated by maxima or minima in the derivative curve. The magnitude of the derivative at this point gives the slope of a tangent to the peak. The ratio of the absolute values of the derivative maximum and minimum gives a measure of peak symmetry.

For the purposes of this study, a symmetric peak is defined as that having a front to rear tangent slope ratio of 1 ± 0.2. The highly asymmetric peaks that result from excessive probe concentrations or adsorption, two of the many factors which can cause deviations from Henry's law in the chromatographic column, are not amenable to analysis by the methods outlined here for Gaussian-shaped peaks. The time period between maximum and minimum of the derivative curve can be measured easily and is equal to twice the standard deviation of the peak, as illustrated in Figures VI-1 and VI-6. The above procedure was used to collect information on the center position, standard deviation, and symmetry of the eluted diffusant peaks.

Relative Diffusivity Determinations

As noted earlier, the probes listed in Table VI-5 were studied in the same LPE-containing column. This allows the diffusivity of one probe in LPE to be compared to that of another, irrespective of the method of any calculation of the absolute diffusivity of the probes in the polymer. The experimental data acquired for tridecane in LPE is given in Table VI-6 and can be used to give an indication of typical values of the various parameters utilized in these determinations. The variables p_i, p_o, and t_M are used in the calculation of u_c by equations 23 and 24. The plate height is determined from $w_{\frac{1}{2}}$ and t_R with equation 1 or from w_i and t_R by the following expression:

$$H = \frac{L}{4}\left(\frac{w_i}{t_R}\right)^2 \qquad (25)$$

When values of A and B are available, the plot suggested by equation 15 can be constructed from the data of Table VI-6. The previous annual report [1] contains a more detailed example of the calculation of these two constants from equations 3 and 4 than the abbreviated discussion given here. The values used in calculating $\bar{H}'/u_o$ are given in a footnote to Table VI-6.

Table VI-6

Experimental Data for an IGC Diffusivity Study of Tridecane in Linear Polyethylene at 150 °C

Pressure (Torr)		Time to Maximum (s)		Peak Width (s)		Outlet Velocity	Plate Height	Ordinate	Abscissa
p_i	p_o	t_M	t_R	$w_{1/2}$	w_i	u_o(cm/s)	$\bar{H}$ (cm)	$\bar{H}'/u_o$,(ms)*	$2p_o/(p_i+p_o)$
3160	745.9	4.23	54.6	8.68	7.34	108.2	0.705	6.31	0.3819
2590	745.0	5.29	69.0	9.79	8.34	72.2	0.562	7.44	0.4468
2103	743.4	6.94	90.6	11.10	9.45	46.0	0.419	8.49	0.5224
1827	744.6	8.43	111.0	12.15	10.29	33.6	0.335	8.95	0.5790
1577	745.2	10.78	141.0	13.73	11.68	23.3	0.265	9.56	0.6417

*The following values were used in the calculation of $\bar{H}'/u_o$: L = 154.9 cm, A = 0.0165 cm, B = 0.585 cm^2/s

Plots of $\bar{H}'/u_o$ against the $2p_o/(p_i + p_o)$ term are shown for five diffusants in Figure VI-7. The slopes of these plots provide a value for the C constant needed in a diffusivity determination. These C values are listed in Table VI-7, accompanied by the corresponding value of k for each

Table VI-7

Relative Diffusivity Results for Several Alkanes and BHT in LPE at 150 °C

Probe	C (ms)±σ(%)	k±σ(%)	D_{Probe}	$D_{Probe}/D_{C_{18}}$	D ($10^7 \cdot cm^2/s$)
C_{18}	21.9± 7	119 ±3	0.38 Y	1	2.4
C_{16}	7.8±14	60.9±1	2.05 Y	5.4	13
$2MeC_{15}$	8.7±12	49.0±1	2.25 Y	6.0	14
$7MeC_9$	18 ±11	12.8±1	3.74 Y	9.9	24
C_{13}	12 ± 9	12.1±1	5.74 Y	15.2	36
BHT	9.9±11	32.4±2	2.94 Y	7.8	19

probe as calculated from the data of Table VI-6 by equation 6. This information can then be used to determine a value for the relative diffusivity by the following procedure. Equation 17 can be rearranged to collect all the variables used only to characterize the polymer packing into one term and solved for the diffusivity. The following expression results when this is done:

$$D_s = \frac{k}{C(1 + k)^2} \left(\frac{r^4 m_s \rho}{168.75\ \rho_s} \right)^{\frac{1}{2}} \qquad (26)$$

The first term in the above equation contains the variables which characterize the interactions between the probe and polymer while the square room term consists of variables which describe polymer layer and support

particle characteristics only. These latter variables are constant throughout all determinations with this particular column and this collection of parameters can be abbreviated as the constant Y. The following version of equation 26 is consequently obtained:

$$D_s = \frac{k}{C(1 + k)^2} \cdot Y \qquad (27)$$

This equation was used to determine the probe diffusivity values given in the fourth column of Table VI-7. If one of the probes is selected as a reference, in this instance octadecane, the diffusivity of a probe in the polymer relative to the diffusivity of the reference probe in that polymer can be obtained from a ratio of the respective results from equation 27. These values are given in the fifth column of Table VI-7.

An alternate determination of the relative diffusivity might be based on equation 7. In this instance the following expression would be obtained for D_s:

$$D_s = \frac{k}{C(1 + k)^2} \cdot \frac{2s^2}{3} = \frac{k}{C(1 + k)^2} \cdot Y' \qquad (28)$$

Equations 27 and 28 are identical except for the constants Y and Y', which are derived from different collections of parameters used to describe the distribution of the polymer phase on the support. The numerical front-factor for Y' is identical to that given for Y in column four of Table VI-7 since it depends only on the values of C and k, which are the same for either method. The relative diffusivity results would also be identical as the Y or Y' constant is eliminated by the ratioing method used to obtain this quantity.

An absolute diffusion constant for each probe in the polymer can readily be obtained from the relative diffusivity values if an absolute diffusion coeffi-

cient for any of the probes in that polymer exists. Taking the previously cited value in Table VI-3 for column B of 2.4×10^{-7} cm^2/s for octadecane in LPE at 150 °C as accurate, the absolute diffusivities in column six of Table VI-7 were otained by multiplying the relative diffusion coefficients of column five by this factor.

Future Results

Results on lower molecular weight alkanes, principally isomers of octane and normal decane and tridecane, at temperatures below the LPE melting point will be given in a later report. They will allow a more rigorous evaluation of the IGC relative diffusivity technique as many more absolute diffusivity determinations have been conducted with these compounds. Independent values for the absolute diffusion coefficient of tridecane in LPE will then be available at two temperatures, one below and one above the polymer melting point. By using an appropriate activation energy to extrapolate one of the results and making allowances for the expected effects of polymer crystallinity on the diffusion coefficient, a direct comparison of the two results will be possible. Unfortunately, it is not possible to study the alkanes from octane to octadecane at a single temperature due to the great differences in volatility among these compounds. This necessitates the temperature extrapolation for a common probe described above as a means of connecting the two bodies of data collected at different temperatures and allowing for a critical evaluation of the method. Additional results for BHT at lower temperatures will also be provided.

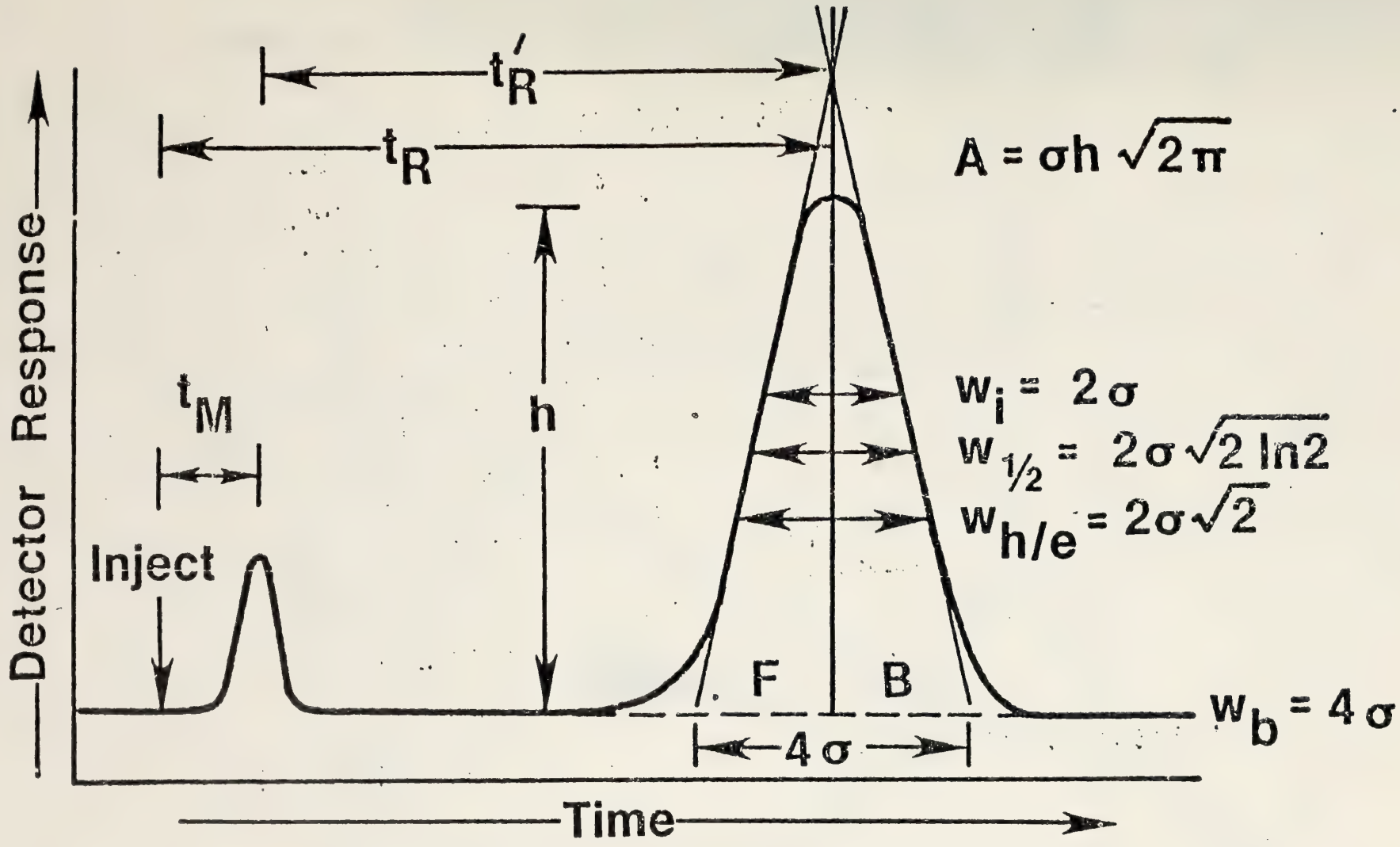


Figure VI-1: Elution chromatogram schematic showing a marker peak at t_M and a Gaussian probe peak at t_R. Various methods of determining the standard deviation σ are indicated.

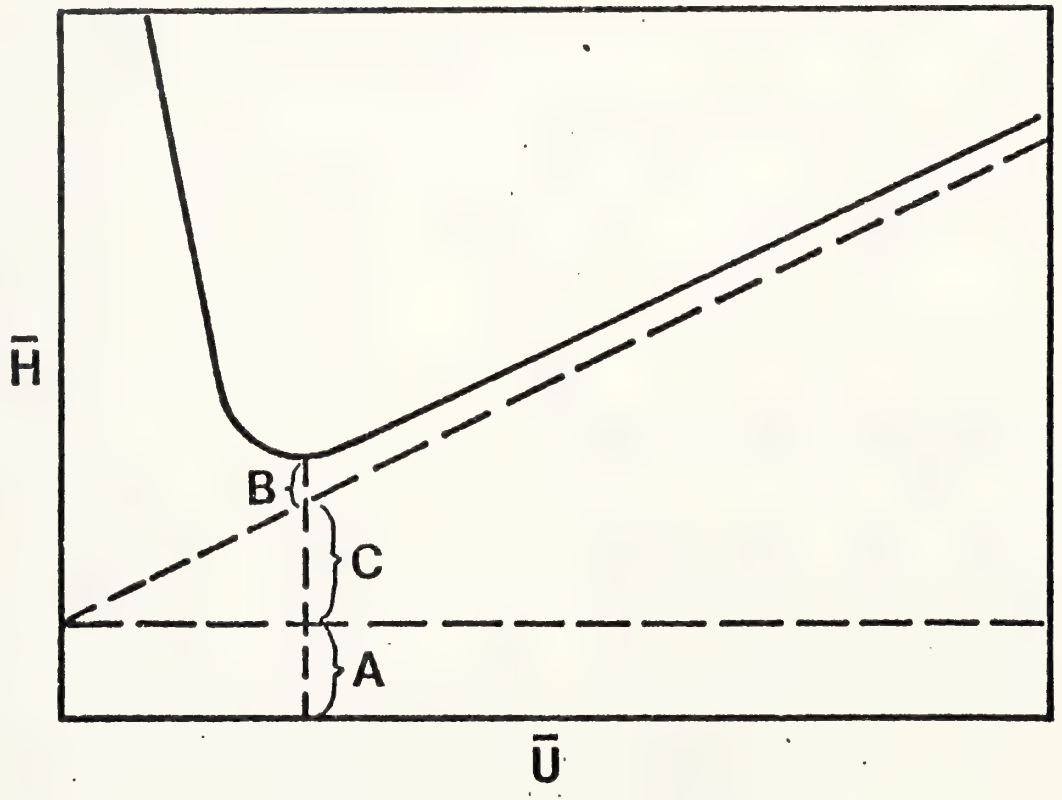


Figure VI-2: van Deemter plot of the height equivalent to a theoretical plate against the average carrier gas flow velocity.

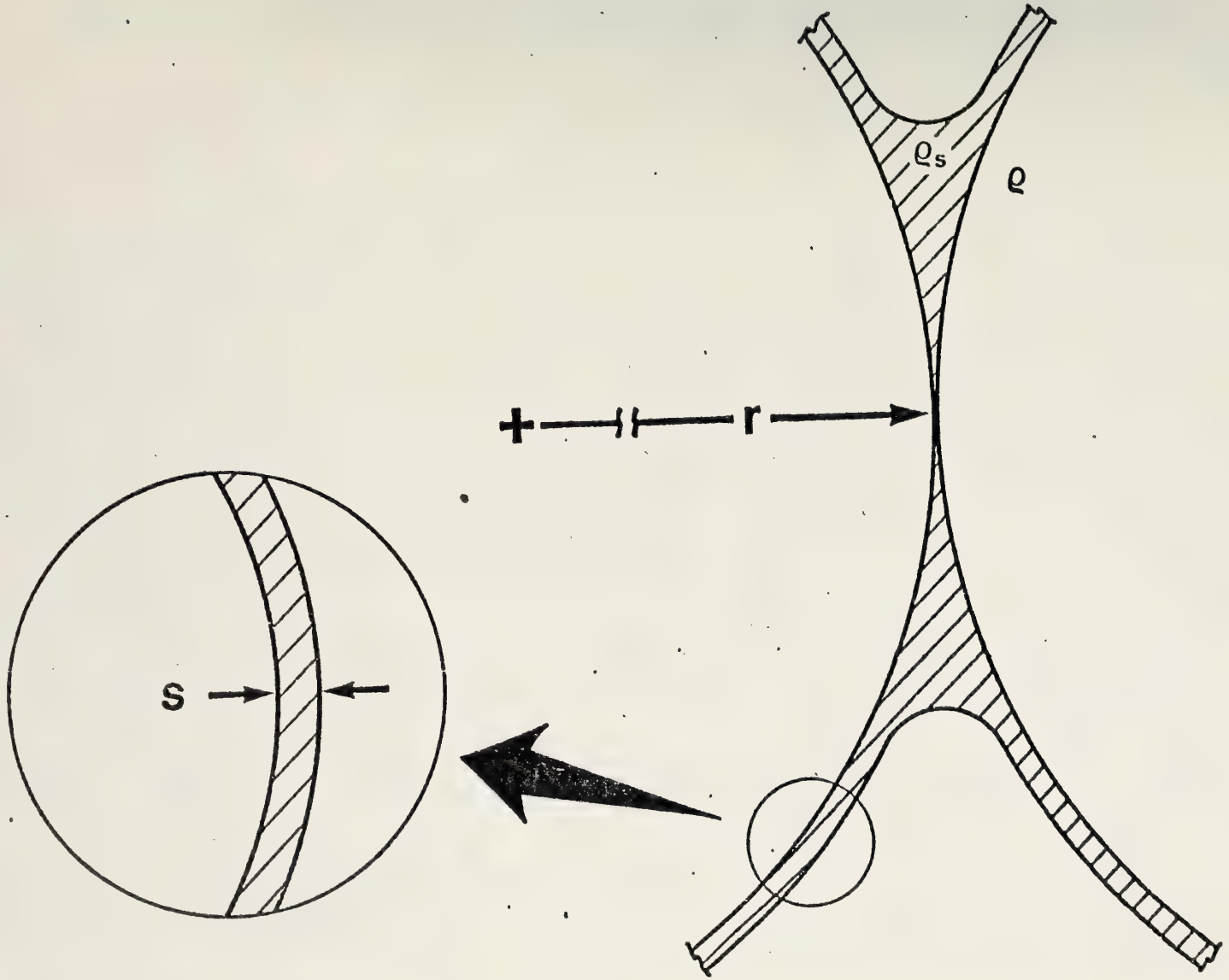


Figure VI-3: Illustration of the possible polymer phase geometries within an IGC column containing a glass bead support.

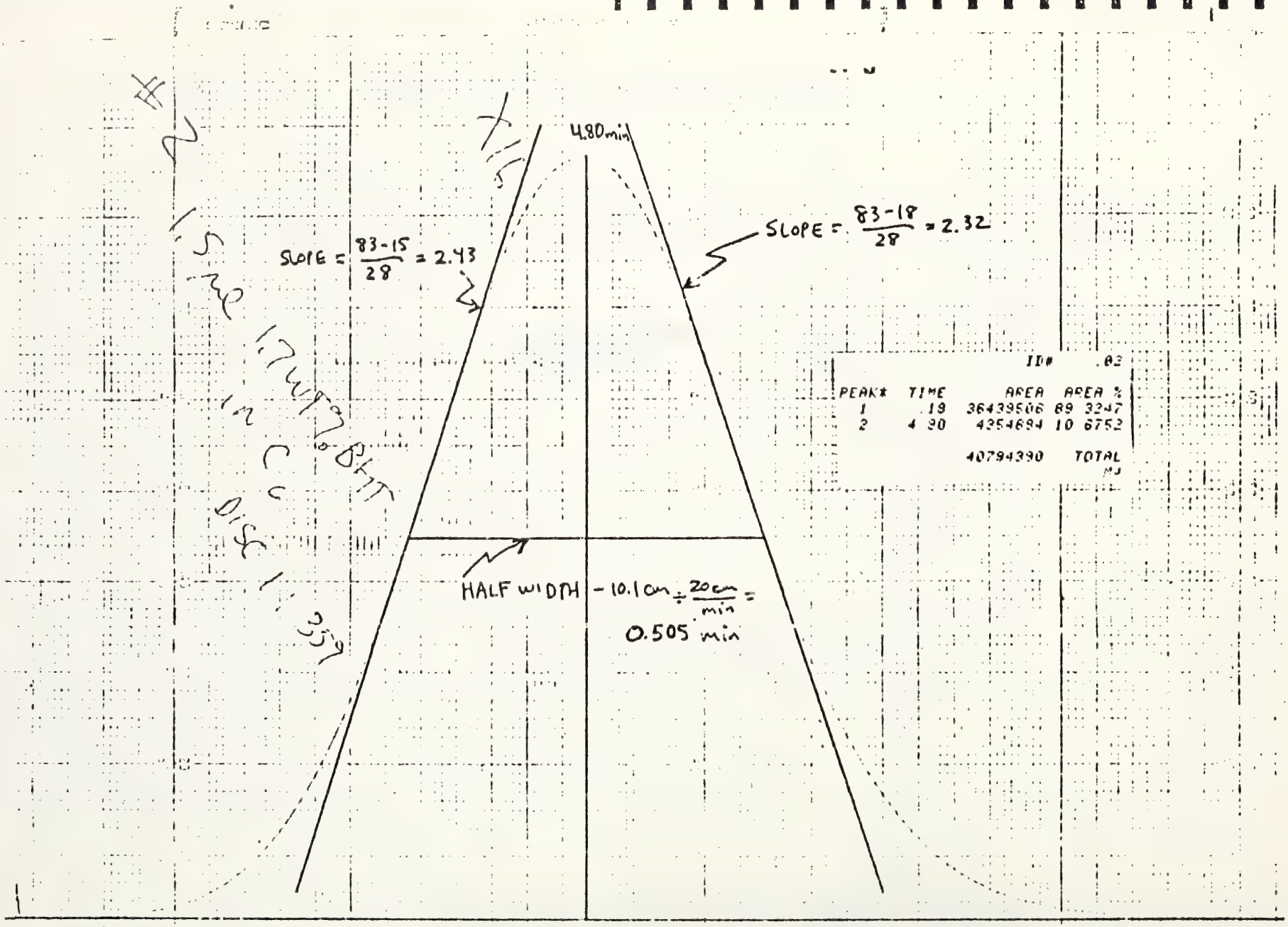


Figure VI-4: Typical strip chart recorder output of a probe peak showing the methods for determining the width at half maximum and tangent slopes.

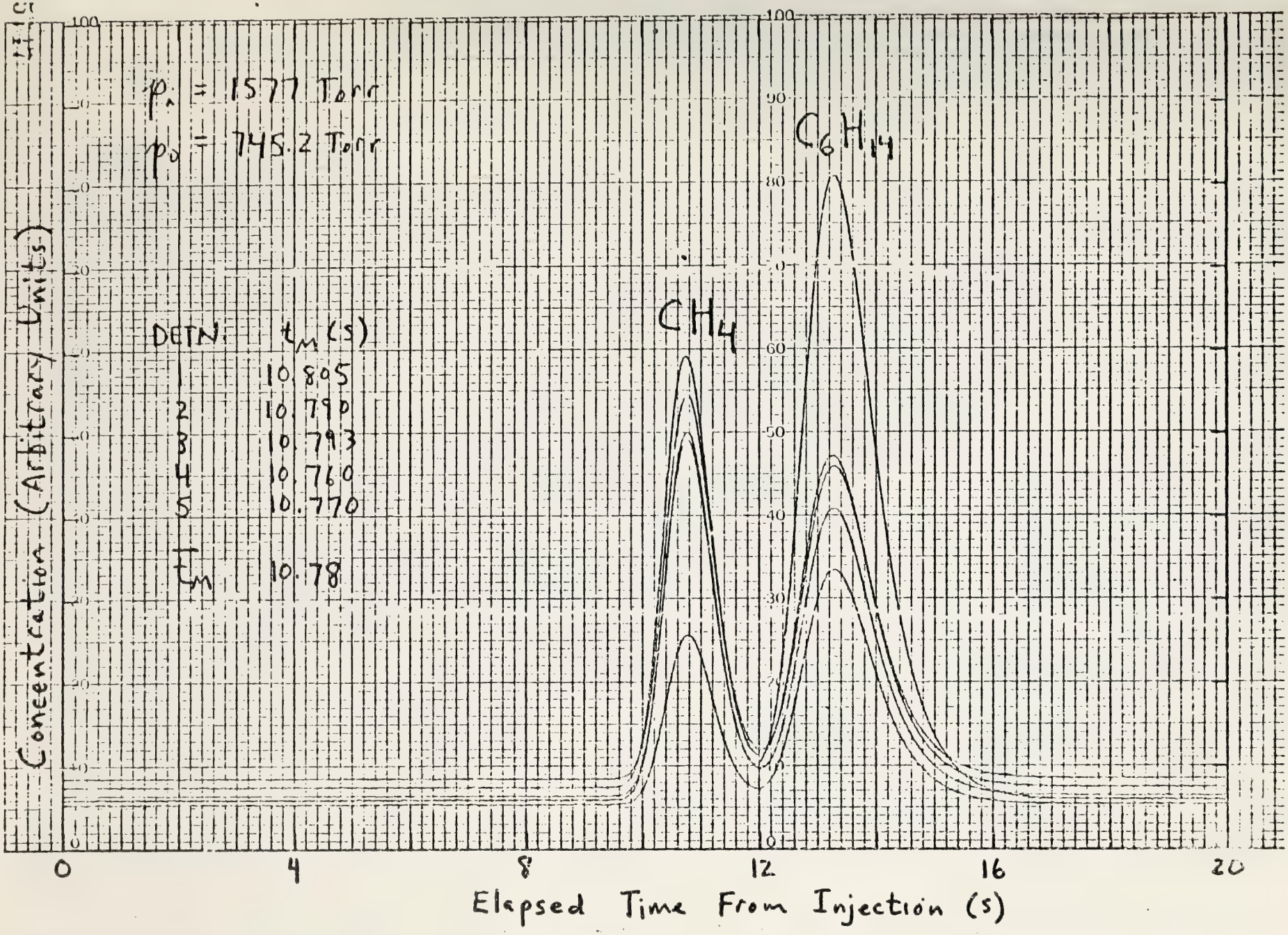


Figure VI-5: High speed chart record of five determinations of t_M with methane as the marker. A hexane solvent peak is also present.

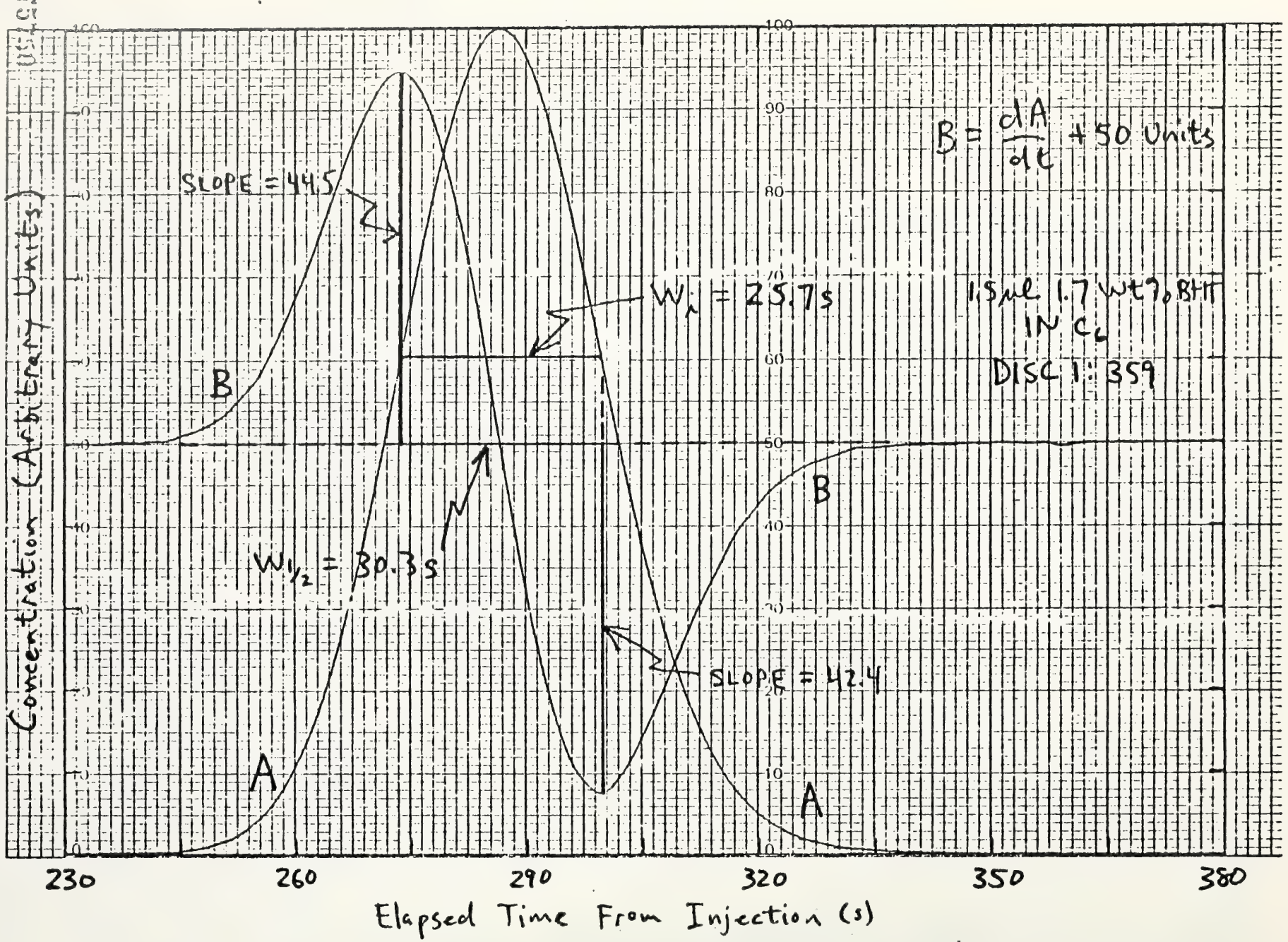


Figure VI-6: Typical high speed chart record of a probe peak (curve A) and first time derivative (curve B) showing the methods for determining the width at half maximum, width at the inflection points, and tangent slopes.

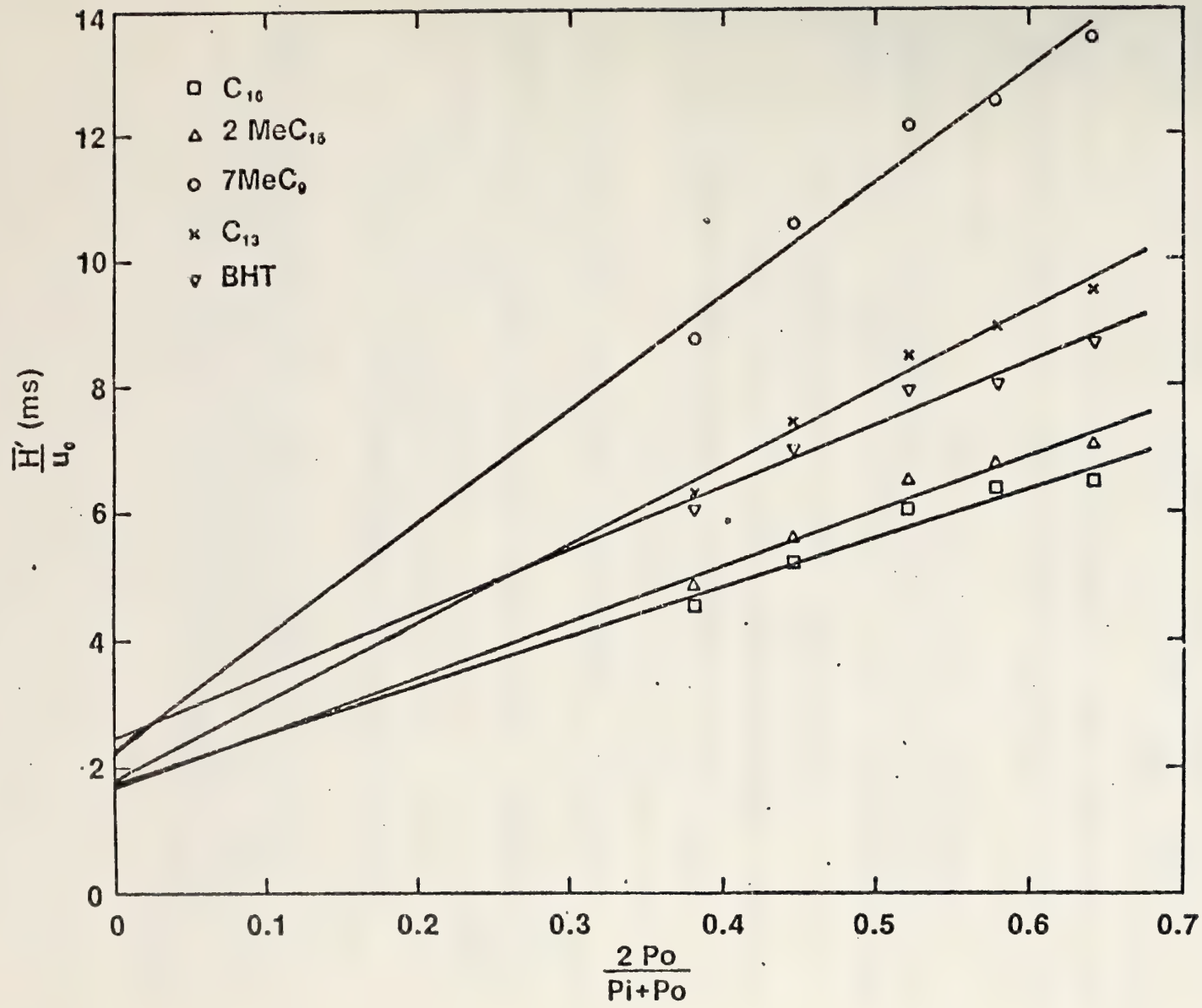


Figure VI-7: Plot of $\bar{H}'/u_o$ vs $2p_o/(p_i + p_o)$ suggested by equation 15 for five diffusants in LPE at 150 °C.

References and Notes

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16. Certain commercial equipment, instruments, or materials are identified in this paper in order to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

VII. A Simplified Migration Decision Tree

One of the most important parameters in indirect food additive regulation is the maximum allowable concentration or a critical concentration of the species of concern in food, C^*. This value is based upon toxiological studies and from the fractional amount of total food consumed, that would be in contact with the packaging material of concern.

Acceptable migration would be the case in which an upper bound level of migration for the maximum time and temperature for storage and usage, based upon either actual tests of sound estimations, is less than the critical or threshold level.

To this end, we have exemplified and simplified our decision tree described earlier (NBSIR 79-1779) as a flow chart shwon in Figure VII-1.

1. Load Limited Migration

In the ultimate case, all the migrant of concern moves from the packaging material into food. The concentration of the migrant in food is:

$$C = \frac{V_p C_o}{V_s}$$

where C_o is the original concentration of the migrant in the packaging material, V_p and V_s are the volumes of the packaging material and food or solvent respectively. Migration is acceptable if this concentration is less than the critical concentration, C^*.

In general, 10 g food is considered in contact with 1 in^2 (6.45 cm^2) of the packaging material (CRF Title 21, Part 21, Part 177). In other words, by approximating the density of foods as 1 gcm^{-3}, the ratio of the volumes of the packaging material to food V_p/V_s is 0.645 ℓ where ℓ is the thickness of the packaging material in cm. Commonly this ratio is less than 1:40 or the thickness of the packaging material is less than 0.04 cm.

Therefore, the migration level is acceptable if the following conditions are met:

$$C_o < \frac{V_s}{V_p} C^* \qquad \text{for all cases,}$$

or

$$C_o < \frac{1.53}{\ell} C^* \qquad \text{if no less than 10 g of food is in contact with 6.45 } cm^2 \text{ of packaging material,}$$

or

$$C_o < 40C^* . \qquad \text{If } V_p \text{ is less than 1/40 of } V_s.$$

2. Solubility Limited Migration

For the case in which the loading of the migrant of concern is greater than the above limit, the saturation solubility C_{sat} of the migrant in the particular type of food or food simulant is examined in order to find out whether the saturation solubility is less than the critical concentration. Special attention should be given to cases where surfactant or emulsification action may tend to increase the actual migrant concentration in food beyond the saturation concentration. The migration level is acceptabe if

$$C_{sat} < C^* .$$

3. Partition Limited Migration

If both the loading and the solubility exceed the limiting threshold, then the partitioning of the migrant between the packaging material and the food or the simulant should be examined. The partition coefficient k is defined as the quotient of the activities, a, of the migrant in the food and in the polymer at equilibrium. It may also be approximated by the ratio of the solubilities in the solvent and in the polymer,

$$k = \frac{1}{K} = \frac{a_s}{a_p} \simeq \frac{C_{sat}}{C_{p,sat}}$$

By defining α as the ratio of the amount of migrant in the solvent, M_∞, versus that in the polymer, $M_{p\infty}$, at equilibrium

$$\alpha = \frac{M_\infty}{M_{p\infty}} = \frac{V_s}{V_p} k = \frac{V_s C_\infty}{V_p C_{p\infty}},$$

then the final fraction of original amount of additive migrated,

$$\frac{M_\infty}{M_0} = \frac{\alpha}{1 + \alpha}$$

where M_0 is the original loading of migrant in the polymer. For the final concentration in food or solvent to be less than the threshold,

$$C_\infty = \frac{M_\infty}{V_s} < C^*,$$

or

$$\frac{\alpha}{1 + \alpha} \frac{V_p}{V_s} C_0 < C^*,$$

it requires that

$$C_0 < \left(\frac{V_s}{V_p} + K \right) C^*.$$

Thus step 1 is just a special case of step 3.

In the case that the partition coefficient or the saturation concentration of the migrant in the polymer is unknown or difficult to determine, the partition coefficient may be assigned a value as in our previous reports (NBSIR 79-1598 and 79-1779)

$$\ell nk = \ell nC_{sat} + \chi_p^{\infty} + 1 = \ell nC_{sat} + 2$$

In general, χ_p^{∞} is in the range of 0 to 2. Thus

$$k < 20\ C_{sat.}$$

This assigns a solubility of $C_{p,sat}$ of > 0.05. Therefore the requirement is simplified as,

$$C_o < (K + 40)\ C^*,$$

or

$$C_o < \frac{1}{20C_{sat}} + 40 \quad C^*$$

However, this simplification is applicable only when the saturated solubility in the food or solvent is relatively low and the solubility in the polymer relatively high.

4. Diffusion Limited Migration

When the equilibrium properties such as the additive loading in the polymer, the solubility of the additive in the solvent, and the partitioning of the additive between the polymer and solvent all yield too high a final concentration of the additive in the food or the solvent beyond the threshold concentration C^*, then it is necessary to find out kinetically whether, under the particular storage condition and in the limited storage time, the amount of the additive migrated would produce an additive concentration in the solvent less than that of the threshold limit. The kinetics of migration depends upon additive, polymer, and solvent combinations, as well as effects of temperature and stirring. The combination of additive, polymer, and solvent or food is the most important factor influencing the diffusion coefficient. This diffusion coefficient is also dependent upon temperature, with an activation

energy in the order of 10-20 kcal/mol for polymers in the rubbery state. A further relatively minor influence in comparison to the above factors may be observed due to the changes in the degrees of crystallinity and molecular weights of the polymer. Stirring speeds up the approach of an equilibrium condition.

If the migration is kinetically limited, i.e. much less than half of additive is migrated, then we are only interested in the short time behavior; otherwise, the estimation of total migration from step 1 would be sufficient.

For a single-sided extraction, at t when $M_t/M_\infty < 0.5$, we may apply the simple equation

$$\frac{M_t}{M_\infty} = 2\left(\frac{Dt}{\pi}\right)^{1/2}\frac{1}{\ell}$$

In other words

$$\frac{M_t}{A} = 2\left(\frac{Dt}{\pi}\right)^{1/2} C_o,$$

or

$$C_t = 2\left(\frac{Dt}{\pi}\right)^{1/2}\frac{A}{V_s}\, C_o,$$

where ℓ is the thickness of the film and A is the area of contact. For an upper limit, D is assigned the value of the diffusion coefficient measured on the polymer swollen by the solvent concerned. In the upper bound case, all migrants are assumed to be able to migrate from the polymer into solvent, i.e., $M_\infty = M_o = V_p C_o$. If partitioning exists, M_∞ should be reduced from M_o according to that described in step 3.

By assuming a storage time, t, of 1 year (3.15×10^7 s) and a container thickness of 0.04 cm (calculated from a food to container contact area of 10 g/in^2 and a container to food weight ratio of 1:40), one may obtain

$$M_t/M_\infty \cong 1.6 \times 10^5\, D^{1/2},$$

or

$$M_t/A \cong 6300\, D^{1/2} C_o,$$

or

$$C_t \cong 4100\ D^{1/2} C_o.$$

For $M_t/M_\infty = 0.5$, a diffusion coefficient of $D = 10^{-11}\ cm^2 s^{-1}$ is required to meet the threshold limit. Therfore, with the above mentioned storage conditions, only in the cases where D is less $10^{-11}\ cm^2 s^{-1}$ will diffusion limited migration be important enough to be considered. Otherwise equilibrium conditions should be used for estimation. For thinner packaging materials, D should be even less or at less than $6.2 \times 10^{-9} \ell^2 cm^2 s^{-1}$ in order for the kinetic criteria for migration to apply.

For polyolefins, the glass transition temperature is lower than -20 °C. Hence, the semicrystalline solid polymers are, in general, utilized in the condition of mixed rubbery (amorhpous portion) and crystalline states. It is usually assumed that the additive migration occurs in the amorphous region. The diffusion coefficients of migrant for the rubbery state are generally many orders of magnitude higher than those for the glassy state. For oligomers up to $n\text{-}C_{32}H_{66}$ and anti-oxidant molecules such as BHT, the apparent diffusion coefficients into either corn oil, triglycerides or ethanol are near or greater than $10^{-11} cm^2 s^{-1}$ above 30 °C. The influence of solvent, temperature, and crystallinity on the diffusion coefficients of BHT in polyethylene have been summarized earlier in this report. Therefore, for polyolefins, the diffusion limited case exists for these migrants and solvents only at a storage temperature lower than ambient, or at a much shorter storage time (a 10-fold reduction in the amount migrated requires a 100-fold reduction in time), or for a very thick container. The diffusion limited case may also exist for extraction with poor solvents for the migrant. However, in the case with poor solvents, the solubility limit or partition limit requirements may often suffice.

Fig. VII-1. A Simplified Additive Migration Decision Flow Chart

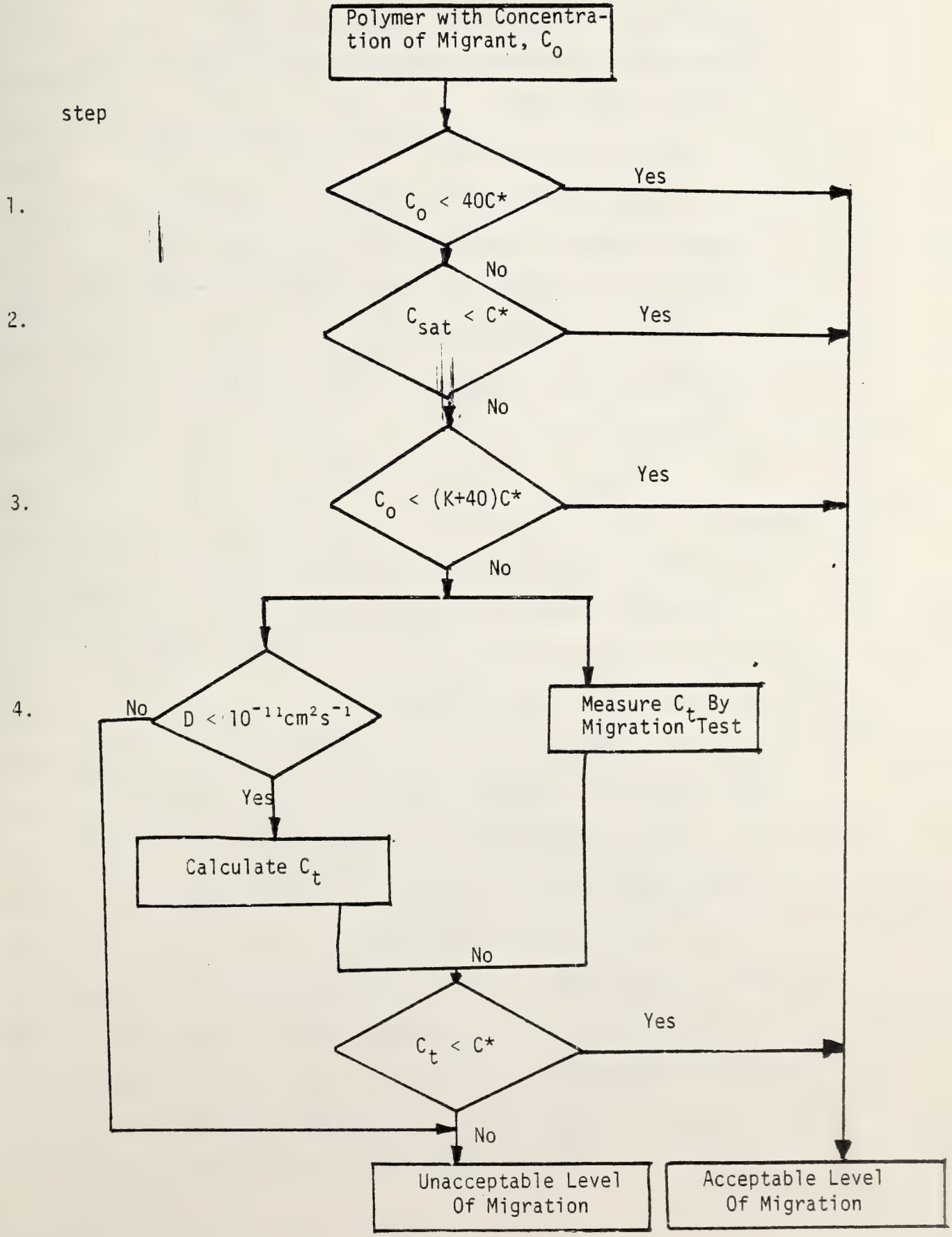

Figure VII-1. (Continued)

Glossary:

C_o - Original concentration of migrant in polymer.

C* - Critical or acceptable concentration of migrant in food or solvent of concern.

C_{sat} - Solubility of migrant in food or solvent of concern.

K - Distribution or partition coefficient of migrant in polymer and in food or solvent at equilibrium, C_{poly}/C_{solv}.

D - Apparent diffusion coefficient of migrant in polymer chain by food or solvent of concern.

C_t - Concentration of migrant in food or solvent after contact time t.

Notes:

1. This flow chart is based upon the assumption of a volume ratio of packaging material/food of 1:40 or 10 g of food are in contact with 1 in^2 or 6.45 cm^2 of packing material. Consult text for other conditions.
2. Along the decision or branching points, move to the next step if the parameter in the particular step is unknown or not determined, the particular step may be skipped and the criteria of the next step will be tested.

VIII. Simulating Solvents

Within the limited temperature range of food utilization and storage, solvent is the single most important parameter effecting both the amount of migrant extractable and the diffusion coefficient of the migrant, acting through its solubilities in and its swelling action upon the polymer.

By correlating diffusion coefficients in other solvents to that in one of the solvents, e.g. ethanol, while keeping all other parameters constant, it is possible to reduce the large spread of diffusion coefficients of the order of 10^8 to within a factor of 5 or less.

For partitioning or low solubility solvents, the correlations depend not only on the solvent but also on the migrant and/or the polymer. However, for solvents having moderate solubilities toward the migrant, the correlation seems to be independent of migrant, polymer or temperature.

The most significant correlations are those found for pure triglycerides and ethanol as food oil simulants and that for the accelerating solvent, n-heptane. As shown in Figure VIII-I, the diffusion coefficients of migrants (n-octadecane, n-dotriacontane or BHT) moving from polyolefins (LPE, BPE, PP) or E-VA copolymers into either tributyrin, trioctanoin or synthetic triglyceride mixture HB307 at either 30 or 60 °C are almost the same as the corresponding diffusion coefficient in corn oil. The diffusion coefficients in the pure triglycerides are slightly higher than that in corn oil with a ratio of D(pure triglycerides)/D(corn oil) less than 1.5 over most of the range studied. Ethanol seems to behave almost identically to the lower members of pure triglycerides in its extraction behavior as shown in Figure VIII-2. However the correlation for the data of ethanol extractions shows more scatter than that for triglycerides within a factor of less than 3 or less.

From the above observations, either ethanol or low members of pure triglycerides may be used successfully for most occasions as food oil simulants, regardless of dissimilarities in viscosities, solvation power for the migrants, and swelling power for the polymers.

The accelerating action of n-heptane over that of food oil has long been recognized. The amount extractable by food oil was sometimes considered to be 1/5 of that by n-heptane. However we found that no constant factor will describe this accelerating action. Beside the differences in solubilities and in partition coefficents, the accelerating power of n-heptane is clearly demonstrated in Figure VIII-3, where diffusion coefficients in n-heptane and in triglycerides (including corn oil) are plotted against those in ethanol for identical test samples and conditions. Regardless of polymer, migrant and temperature, the accerating power is greater at low diffusion coefficients than that at high diffusion coefficients. While, at D(ethanol) around 10^{-7} cm^2s^{-1}, accelerating power is greater at low diffusion coefficients than that at 1000 at D(ethanol) around 10^{-11} or $10^{-12}cm^2s^{-1}$.

The accelerating action of n-heptane compared to that of ethanol (and that of triglycerides), coupled with the differences in solubilities of oligomers of polyolefins, has dramatic effects on the total extractables of polyolefins. We, therefore, subjected large quantities (50 g) of the raw polymer stocks of SRM 1475 (LPE) and SRM 1476 (LPE) to extraction by 500 ml of ethanol n-heptane at 70 °C for 160 days with occasional shaking. By assigning a minimum diffusion coefficient of about 10^{-9} cm^2s^{-1} for n-$C_{32}H_{66}$ and a pellet radius of 0.1 cm, the effective time $T = Dt/\ell^2$ is 1.4. Thus according to the generalized solution for the diffusion equation, the extraction should be at least 95% complete. The results of the 160-day extractions are listed in

Table VIII-I. For each polymer, about 6 to 8 times as much of polymer fraction was extracted by n-heptane than by ethanol.

The extracts were then subjected to gel permeation or size exclusion chromatographic analysis by Roger C. Snyder of FDA to find out their molecular weight distributions, as summarized in Table VIII-2 and shown in Figure VIII-4 for linear polyethylene SRM 1475 extracts, respectively. The molecular weight scales were calibrated by means of analyzing five NBS polyethylene standard reference materials, three n-alkanes (C_{10}, C_{20}, C_{44}) and test mixtures containing known amounts of n-alkanes from C_6 to C_{44}. The molecular weight scale for branched polyethylene is only approximately correct, however it should be sufficient for comparison purposes.

The extracts from the linear polyethylene show rather normal symmetrical distributions with peaks of molecular weight centering at about 300 for ethanol and at about 800 for n-heptane extracts. Such results are expected from the practice of molecular weight fractionation by solvents of different solubility power. On the low molecular weight side, e.g., n-$C_{18}H_{38}$, there is a large enough solubility or even total miscibility of the oligomer fraction in both solvents, such that almost all of the low molecular weight fraction will be dissolved by the extraction processes, cf. labels A in Figures VIII-4 and VIII-5. As molecular weight becomes higher, e.g., n-$C_{32}H_{66}$, the solubility in the solvent, especially in ethanol, decreases which causes a partitioning of the particular component between the polymer and the extracting solvent to occur, cf. labels B in Figures VIII-4 and VIII-5. The partitioning of n-$C_{32}H_{66}$ has been confirmed by extraction experiments with ethanol. The diffusion coefficients for larger molecules also drop significantly. Thus the combination of the effects of solubility, partitioning and diffusion created the shape of the molecular weight distribution curve beyond the peak molecular weight extracted.

A similar comparison for branched polyethylene is seen in Figure VIII-5. The skewed curves are most likely due to the incorrectness of the size versus molecular weight calibration which was based on n-paraffins and linear polyethylene fractions. The peak of apparent molecular weight extracted is about 350 for ethanol and about 3200 for n-heptane extracts.

Therefore, n-heptane can not only accelerate the diffusion process but also remove high molecular species of oligomers that may be hardly present in ethanol or triglyceride extracts.

Table VIII-1

Extraction of Polyethylenes

by solvents at 70°C for 160 days

Solvent	Fraction Extracted	
	LPE SRM 1475	BPE SRM 1476
Ethanol	0.0008	0.0023
n-Heptane	0.0047	0.018

Table VIII-2

Molecular Weight Distributions of Ethanol and

n-Heptane Extractions of Polyethylenes

	$M_n : M_w$	
Solvent	LPE SRM 1475	BPE SRM 1476
Ethanol	250 : 310	310 : 410
n-Heptane	560 : 1020	620 : 3000

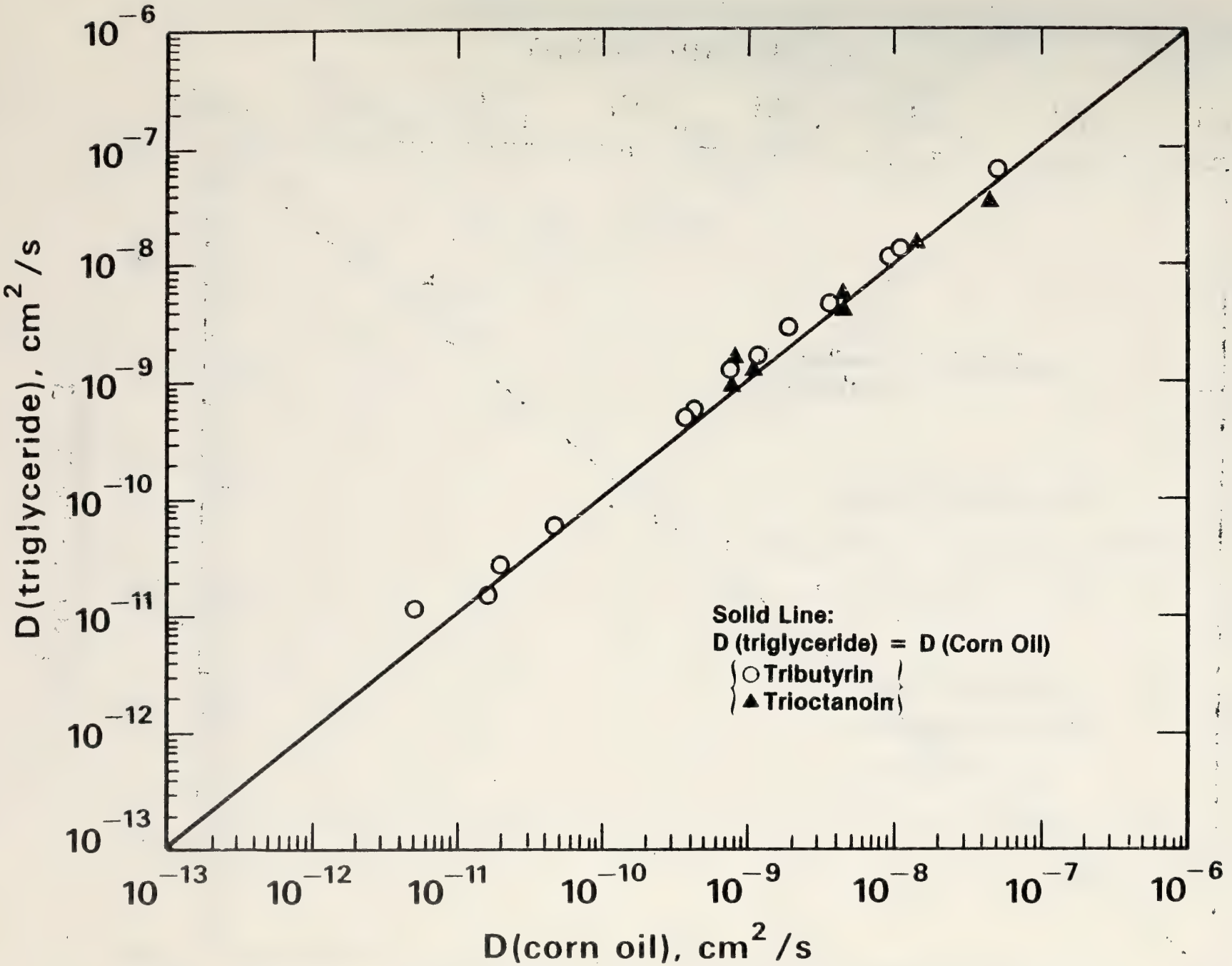

Figure VIII-1 Comparison of Diffusion Coefficients in Triglycerides and in Corn Oil

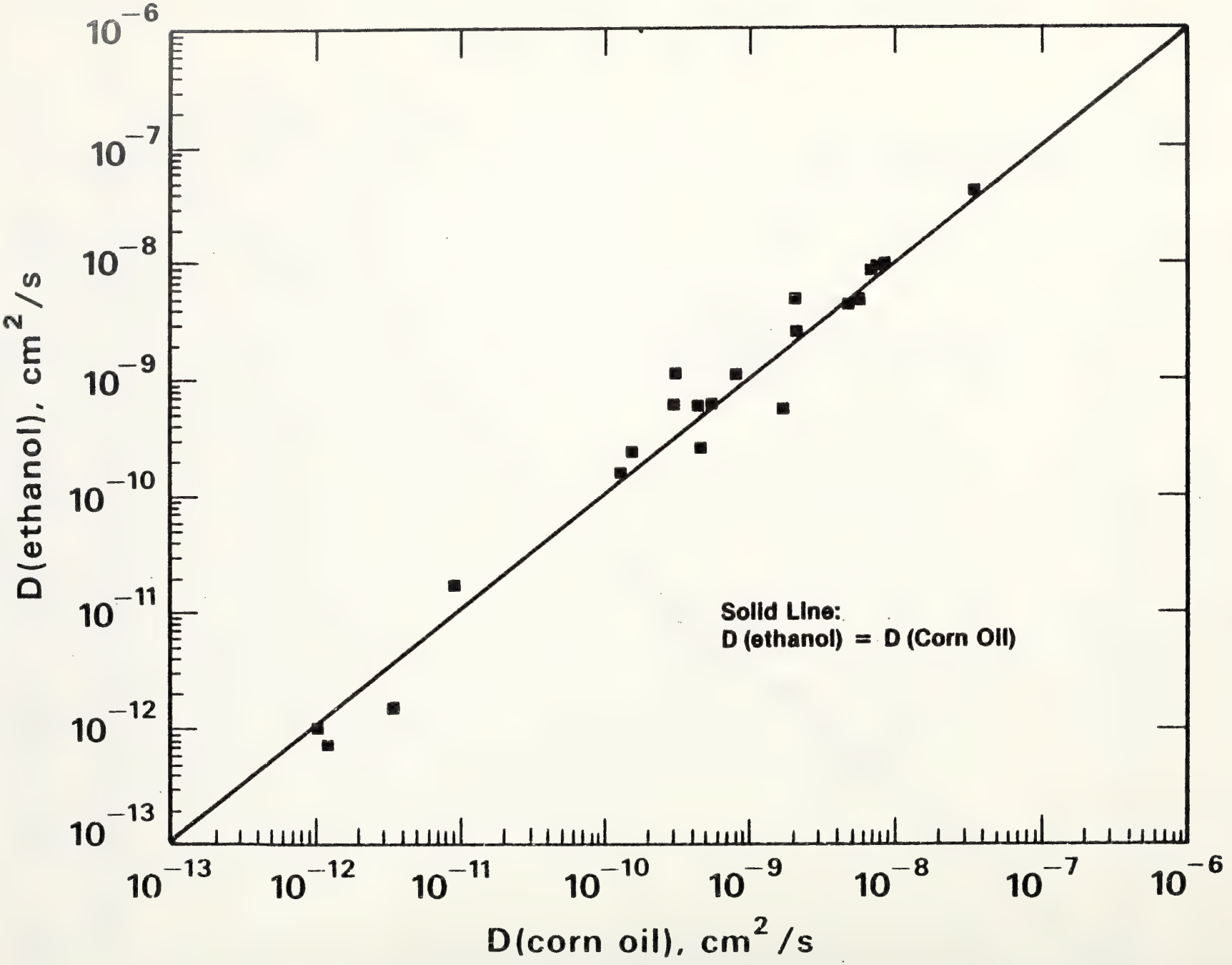

Figure VIII-2 Comparison of Diffusion Coefficients in Ehanol and in Corn Oil

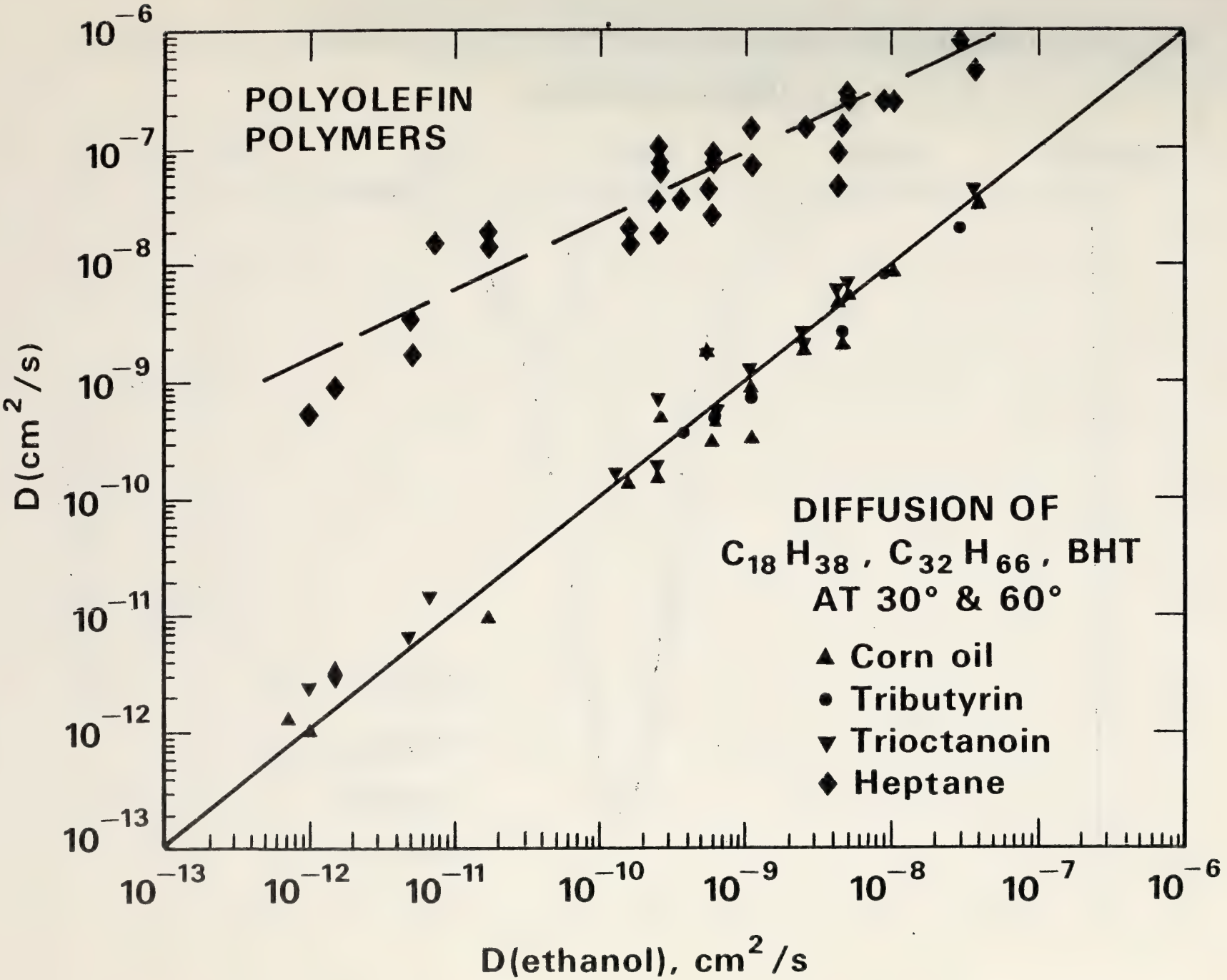

Figure VIII-3 Effect of Accelerating Solvent

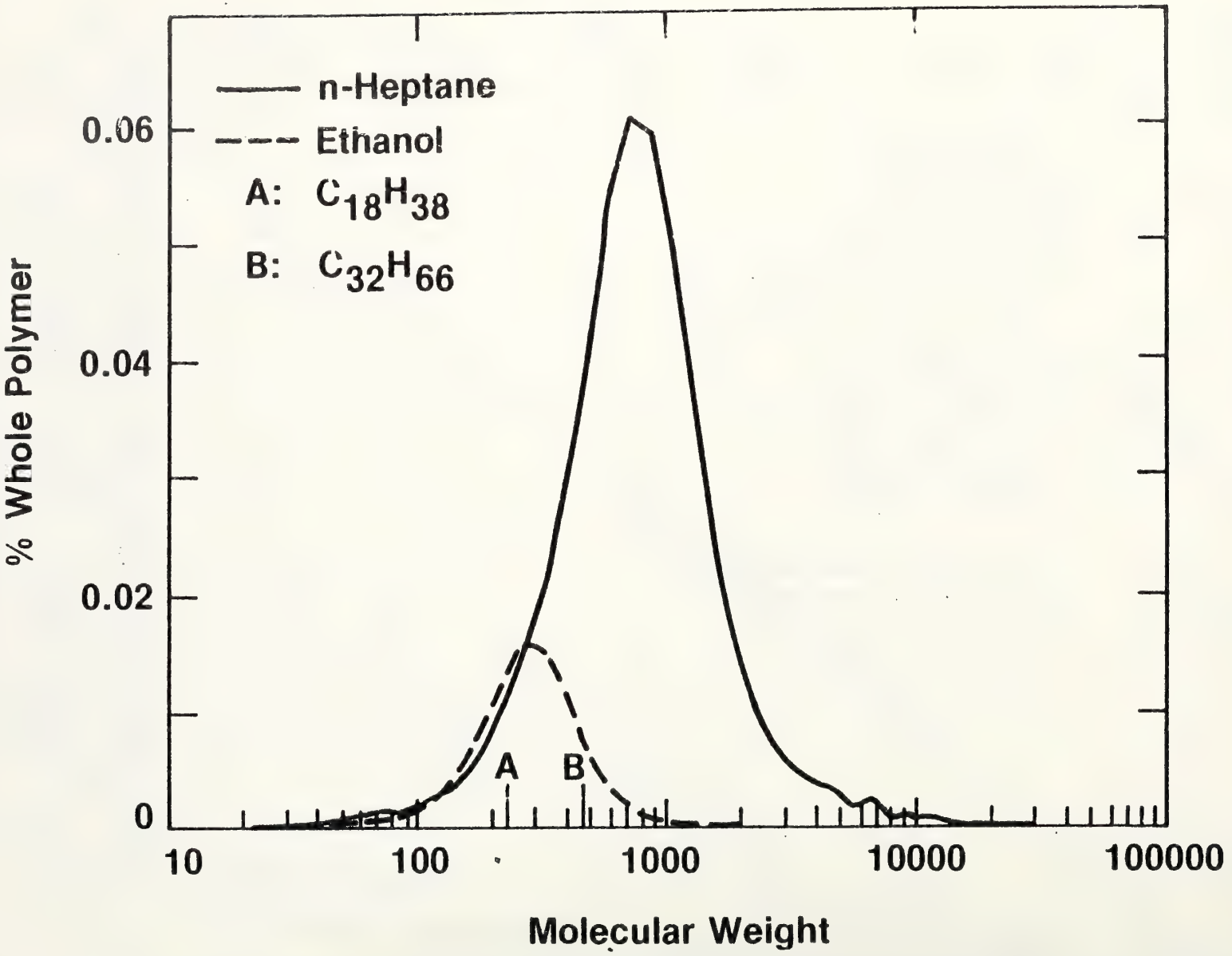

Figure VIII-4 Molecular Weight Distributions of Ethanol and n-Heptane Extracts of LPE

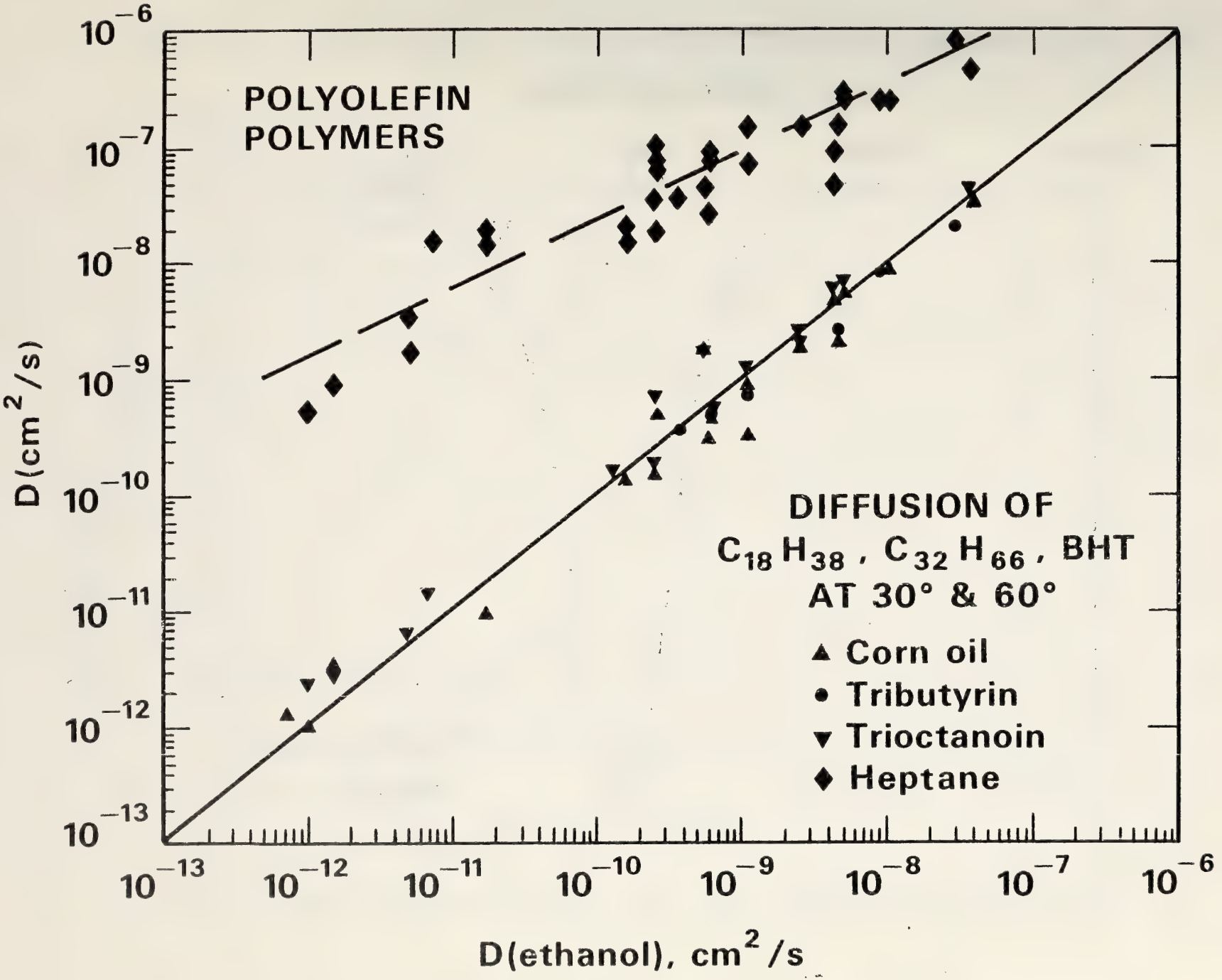

Figure VIII-3 Effect of Accelerating Solvent

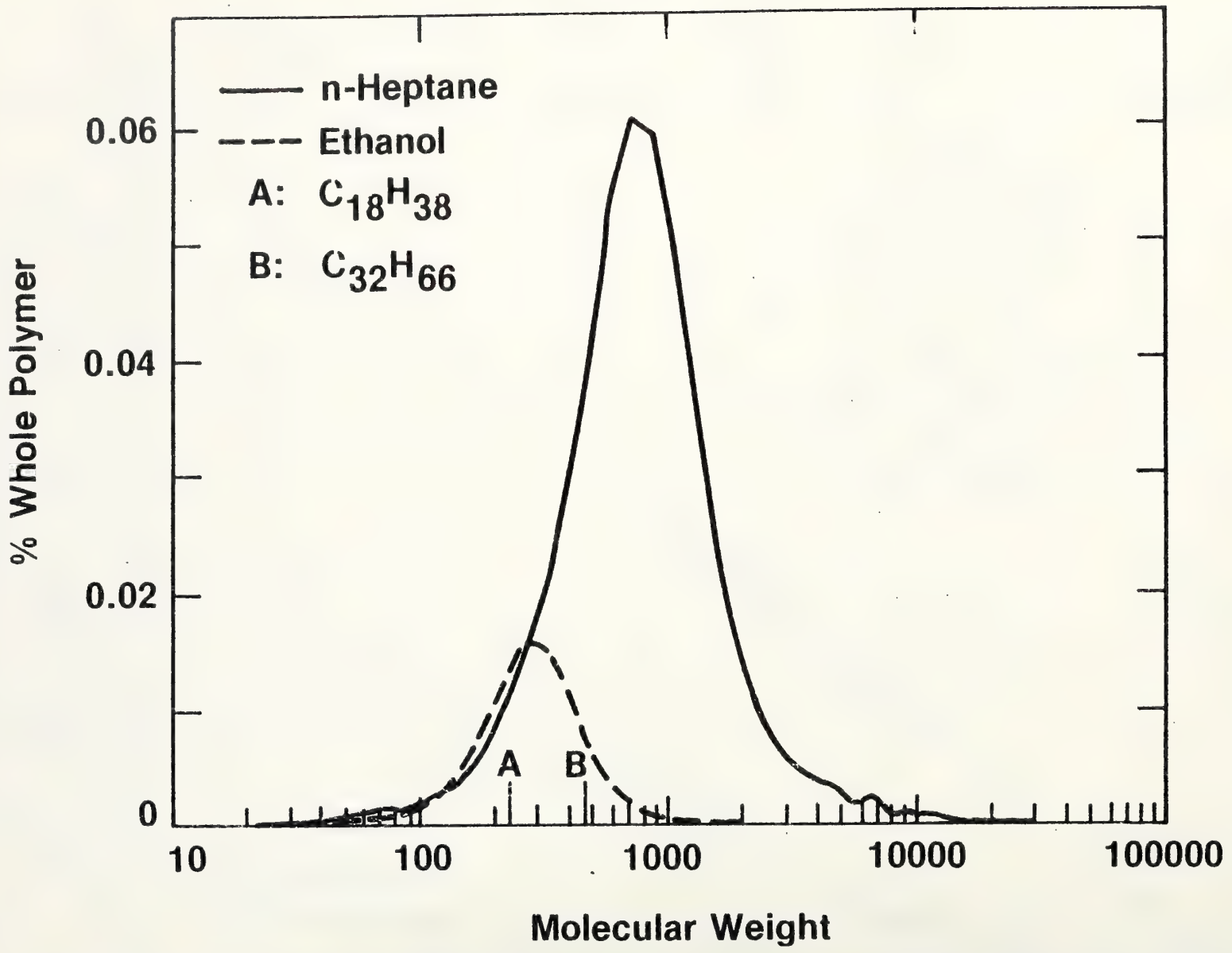

Figure VIII-4 Molecular Weight Distributions of Ethanol and n-Heptane Extracts of LPE

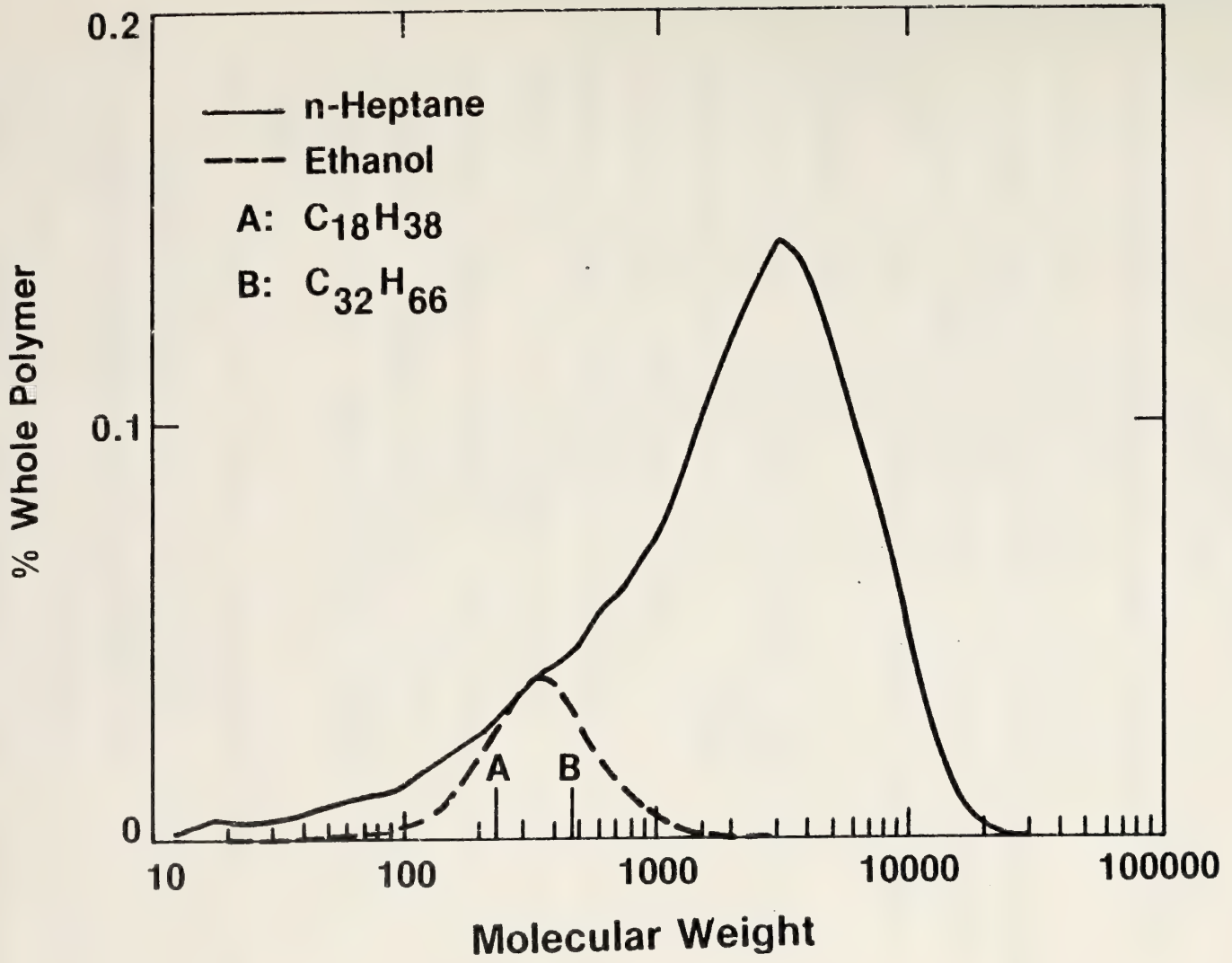

Figure VIII-5 Molecular Weight Distributions of Ethanol and n-Heptane Extracts of BPE

IX. Summary of Conclusions

* Maximum amount of extractables depends on the original migrant concentration in the polymer, the solubilities and the partition of the migrant in solvent and in polymer.
* Migration behavior is mainly Fickian.
* Diffusion coefficient may be increased by absorption of the solvent or swelling of the polymer by the solvent.
* Activation energies for the change of diffusion coefficient as a function of temperature generally lie between 40 and 200 kJ mol^{-1}. In general, the activation energy is lower at higher diffusion coefficients.
* Lower members of pure triglycerides may be used to simulate the extraction behavior of corn oil in oligomers and anti-oxidants, such as BHT, from polyolefins.
* Anhydrous ethanol may also be considered as food-oil simulant.
* Accelerating action of n-heptane over that of food-oils or oil simulates is more pronounced at lower diffusion coefficients.
* n-Heptane will remove high molecular weight fractions of oligomers which may hardly be present in food oil or oil simulants.
* Diffusion coefficient increases with increased oligomer content.
* Increase of amorphous content in a polyolefin produces a corresponding change in diffusion coefficient.
* The following is the ranking of the importance of the parameters effecting the diffusion coefficient of a migrant from polymer matrix into surrounding media:

Solvent > Temperature (limited range) > Swelling
> Migrant Concentration > Amorphous content.

NBSIR 82-2472

Migration of Low Molecular Weight Additives in Polyolefins and Copolymers

X. Appendix

Numerical Data of Migration of Low Molecular Weight Additives from Polyolefins and Copolymers

Experimental Run Designations--cf page II-6, Tables II-4 and II-5

110300
LPE/C18/CO/30C/L

t, h	Mt/Mo
0.033	0.0055
0.1	0.00296
0.167	0.00396
0.333	0.00462
0.5	0.0115
1.17	0.0202
2	0.028
4	0.0422
5.5	0.0494
7	0.0556
30.8	0.103
71.3	0.142
125	0.175
289	0.245
456	0.295
511	0.314
775	0.372
966	0.412
1585	0.505
2164	0.572
2857	0.634
3625	0.681
4132	0.71
4825	0.739
5523	0.765
6268	0.789
6940	0.804
7657	0.815
8213	0.824
8737	0.822

110600
LPE/C18/CO/60C/L

t, h	Mt/Mo
0.017	0.0104
0.033	0.019
0.067	0.0269
0.133	0.0378
0.25	0.056
0.5	0.0855
1	0.125
1.5	0.15
2.5	0.185
4	0.227
6	0.268
8	0.304
23.5	0.47
31	0.524
48.5	0.631
54	0.651
120	0.834
128	0.85
198	0.914
289	0.959
457	0.985
725	0.996
965	0.981

120600
LPE/C18/EN/60C/L

t, h	Mt/Mo
0.017	0.0149
0.033	0.0185
0.067	0.0287
0.133	0.0456
0.25	0.0693
0.5	0.0996
1	0.135
1.5	0.159
2.5	0.197
4	0.239
5.5	0.275
8	0.323
24	0.527
55.8	0.745
120	0.92
216	0.98
384	1.06
384	0.997
558	0.961
558	0.957

125600
LPE/C18/.5EN/60C/L(1)

t, h	Mt/Mo
0.017	9.16E-4
0.033	0.00176
0.067	0.0028
0.133	0.00485
0.25	0.00821
0.5	0.0147
1	0.0263
1.5	0.0342
2.5	0.0471
4	0.0571
5.5	0.0635
7	0.0677
23.8	0.0683

125602
LPE/C18/.5EN/60C/L(2)

t, h	Mt/Mo
0.017	6.69E-4
0.033	0.00126
0.067	0.00241
0.133	0.00438
0.25	0.00741
0.5	0.015
1	0.0263
2	0.0434
3.5	0.0609
20.5	0.0964
44.5	0.0962

125603
LPE/C18/.5EN/60C/L(3)

t, h	Mt/Mo
0.083	0.00289
0.167	0.00552
0.333	0.01
0.667	0.0174
1	0.0233
1.75	0.0363
4	0.0573
7	0.0723
24.3	0.0992
78.8	0.107
174	0.117

127600
LPE/C18/.7EN/60C/L

t, h	Mt/Mo
0.017	0.00912
0.033	0.0161
0.067	0.0251
0.133	0.0341
0.25	0.0505
0.5	0.0771
1	0.11
1.5	0.133
2.5	0.163
4	0.196
5.5	0.22
7.5	0.252
24.5	0.383
30	0.429
96.5	0.565
147	0.568
196	0.578
264	0.569
344	0.577

129600
LPE/C18/.9EN/60C/L

t, h	Mt/Mo
0.017	0.0172
0.033	0.0215
0.067	0.0299
0.133	0.0443
0.25	0.063
0.5	0.0903
1	0.126
1.5	0.148
2.5	0.182
4	0.221
5.5	0.25
7.5	0.286
23.5	0.456
31.5	0.515
48.5	0.616
54	0.658
121	0.818
171	0.829
220	0.87
289	0.885
386	0.886
625	0.893
893	0.89
1204	0.905

130240
LPE/C18/HP/24C/L

t, h	Mt/Mo
0.1	0.0456
16	0.836
23	0.891
40	0.932
70	0.955
136	0.964
216	0.969
309	0.972
358	0.975
666	0.974

130241
LPE/C18/HP/24C/U

t, h	Mt/Mo
0.025	0.0262
0.05	0.0392
0.1	0.0533
0.25	0.0827
0.5	0.115
1	0.163
2	0.242
4	0.378
8	0.662
28	0.902
72	0.947
151	0.962
245	0.968
294	0.97
438	0.971
462	0.974
512	0.974
579	0.975

130301
LPE/C18/HP/30C/U

t, h	Mt/Mo
0.017	0.0226
0.033	0.0348
0.067	0.0463
0.133	0.0652
0.267	0.0914
0.5	0.123
0.75	0.151
1	0.176
1.5	0.219
2.5	0.295
4	0.402
5.5	0.51
7.5	0.648
24	0.883
31.5	0.903
96	0.946
144	0.954
199	0.959
264	0.962
320	0.964
439	0.967
534	0.968
672	0.97
1033	0.972
1269	0.974
1464	0.974

130601
LPE/C18/HP/60C/U1

t, h	Mt/Mo
0.25	0.265
0.5	0.382
1	0.576
2	0.86
4	0.968
8	0.982
24	0.986
48	0.988
120	0.99
168	0.991

130602
LPE/C18/HP/60C/U2

t, h	Mt/Mo
0.25	0.261
0.5	0.378
1	0.572
2	0.859
4	0.968
8	0.982
24	0.986
48	0.988
120	0.99
168	0.991

140301
LPE/C18/OD/30C/U

t, h	Mt/Mo
0.017	0.00733
0.033	0.0114
0.067	0.0163
0.133	0.0263
0.267	0.0418
0.5	0.0593
0.75	0.0733
1	0.0844
1.5	0.102
2.5	0.126
4	0.157
5.5	0.182
7.5	0.21
24	0.376
31.5	0.437
96	0.865
103	0.885
103	0.887
145	0.936
199	0.949
264	0.955
320	0.958
439	0.962
534	0.964
672	0.967
1033	0.971
1372	0.974
1561	0.974

140601
LPE/C18/OD/60C/U

t, h	Mt/Mo
0.017	0.0273
0.033	0.0462
0.067	0.0688
0.133	0.0962
0.25	0.127
0.5	0.178
1	0.248
2	0.347
4	0.491
6.08	0.61
7.5	0.687
24	0.973

170300
LPE/C18/TO/30C/L

t, h	Mt/Mo
0.017	0.00196
0.033	0.00243
0.067	0.0038
0.133	0.00597
0.25	0.00878
0.5	0.013
1	0.0208
1.5	0.027
2.5	0.0365
4	0.0482
5.5	0.056
7.5	0.0640
24.5	0.117
53.5	0.143
218	0.25
385	0.324
439	0.345
703	0.422
894	0.47
1513	0.583
2092	0.651
2785	0.715
3553	0.768
4061	0.796
4753	0.82
5451	0.841
6196	0.859
6868	0.863
7585	0.864
8140	0.861
8740	0.882

170600
LPE/C18/TO/60C/L

t, h	Mt/Mo
0.017	0.0137
0.033	0.0217
0.067	0.0317
0.133	0.0462
0.25	0.0676
0.5	0.0969
1	0.131
1.5	0.155
2.5	0.192
4	0.228
5.5	0.266
7	0.288
24.5	0.488
30	0.543
96.3	0.827
104	0.841
174	0.924
265	0.966
433	0.978
701	0.988
965	0.978

220240
LPE/C18/EN/24C/L

t, h	Mt/Mo
1	0.114
3	0.161
19.5	0.335
51.5	0.487
116	0.639
195	0.735
288	0.778
337	0.799
387	0.816
505	0.832
648	0.857
820	0.885
1220	0.883
1556	0.9

220241
LPE/C18/EN/24C/U

t, h	Mt/Mo
0.083	0.0165
0.167	0.0234
0.33	0.0352
0.67	0.0518
1	0.0686
2	0.109
4	0.166
8	0.237
24	0.367
48	0.485
78	0.578
216	0.72
409	0.809
745	0.865
1[illegible]	[illegible]02

220300
LPE/C18/EN/30C/L

t, h	Mt/Mo
0.017	0.00744
0.033	0.0127
0.067	0.0173
0.133	0.0252
0.25	0.0384
0.5	0.0577
1	0.0887
1.5	0.114
2.5	0.149
4	0.186
5.5	0.217
7	0.241
23	0.39
31	0.441
48	0.52
55	0.546
120	0.683
128	0.696
168	0.744
223	0.78
294	0.797
384	0.838
535	0.854
720	0.878
1296	0.893
1560	0.904
1966	0.89
2403	0.903
2572	0.912
2572	0.904

220600
LPE/C18/EN/60C/L

t, h	Mt/Mo
0.017	0.05
0.033	0.0708
0.067	0.101
0.133	0.157
0.25	0.239
0.5	0.35
1	0.482
1.5	0.572
2.5	0.698
4	0.808
5.92	0.854
7.92	0.911
23.6	0.968
31	0.966
55.8	0.968
122	0.965
220	0.929
384	0.971
626	0.968
721	0.969
721	0.97
721	0.979

220601
LPE/C18/EN/60C/U

t, h	Mt/Mo
0.017	0.0708
0.05	0.135
0.133	0.232
0.3	0.331
0.55	0.423
1.05	0.543
2	0.688
4	0.84
5.5	0.89
7.5	0.924
24	0.971
55.5	0.98
72	0.981
145	0.983
247	0.986
319	0.986
414	0.987
532	0.988

225600
LPE/C18/.5EN/60C/L(1)

t, h	Mt/Mo
0.017	0.00314
0.033	0.0053
0.067	0.00913
0.133	0.0169
0.25	0.0327
0.5	0.0603
0.75	0.0814
1	0.0971
1.5	0.119
2.5	0.152
4.5	0.164
7.5	0.173
23.7	0.172
31.5	0.172
54.5	0.174
168	0.176
344	0.178

225602
LPE/C18/.5EN/60C/L(2)

t, h	Mt/Mo
23	0.18
65.5	0.178
137	0.182
187	0.186
237	0.21
305	0.176
384	0.181
402	0.179

225603
LPE/C18/.5EN/60C/L(3)

t, h	Mt/Mo
1.15	0.105
2.65	0.146
5.98	0.157
71.3	0.165
168	0.156
240	0.111

225604
LPE/C18/.5EN/60C/L(4)

t, h	Mt/Mo
0.967	0.0639
3.22	0.0906
6.13	0.0954
24	0.0981
47.9	0.0971
268	0.0987
409	0.0978

225605
LPE/C18/.5EN/60C/L(5)

t, h	Mt/Mo
0.167	0.0107
0.333	0.0198
0.667	0.0366
1	0.0518
2	0.0664
4	0.08
5.95	0.0744
22.9	0.0731
29.9	0.0758
94.9	0.0773
195	0.0814

225601
LPE/C18/.5EN/60C/U

t, h	Mt/Mo
0.017	0.00936
0.033	0.0161
0.067	0.0267
0.133	0.0488
0.25	0.0806
0.5	0.119
1	0.191
1.5	0.255
2.5	0.327
4.5	0.409
7.5	0.488
24	0.597
30.5	0.652
120	0.823
361	0.926
698	0.964
1012	0.965
1204	0.978
1347	0.981

229601
LPE/C18/.9EN/60C/U

t, h	Mt/Mo
0.017	0.0669
0.033	0.102
0.083	0.19
0.167	0.249
0.25	0.292
0.5	0.39
1	0.51
2	0.658
4	0.807
5.5	0.862
7.5	0.903
24	0.964
31.5	0.971
48	0.976
120	0.98
193	0.983
222	0.984
295	0.984
390	0.985
508	0.986
519	0.988

230241
LPE/C18/HP/24C/U

t, h	Mt/Mo
0.017	0.0857
0.033	0.124
0.067	0.183
0.133	0.281
0.25	0.458
0.5	0.683
1	0.804
2	0.866
4	0.904
6	0.919
22	0.95
30	0.955
94	0.968
148	0.972
216	0.974
287	0.975

230301
LPE/C18/HP/30C/U

t, h	Mt/Mo
0.017	0.0736
0.033	0.119
0.067	0.19
0.133	0.3
0.25	0.472
0.5	0.715
1	0.812
1.5	0.844
2.5	0.874
4	0.895
5.5	0.906
8.13	0.917
23.8	0.939
47.8	0.949
79.9	0.954
144	0.959
217	0.962
384	0.966
577	0.968
655	0.969

240601
LPE/C18/OD/60C/U

t, h	Mt/Mo
0.25	0.687
0.5	0.922
1	0.978
2	0.984
4	0.987
8	0.99
24	0.992
48	0.993
127	0.994
168	0.995

250300
LPE/C18/0N/30C/L

t, h	Mt/Mo
0.017	0.0132
0.033	0.011
0.067	0.0128
0.133	0.018
0.267	0.0294
0.5	0.0464
1	0.0965
2.03	0.141
3.5	0.189
5	0.233
7.5	0.270
24.7	0.49
30.5	0.541
48.8	0.652
76.8	0.77
145	0.834
241	0.87
337	0.874
484	0.899
649	0.913
676	0.916

250600
LPE/C18/0N/60C/L

t, h	Mt/Mo
0.017	0.0585
0.033	0.0897
0.067	0.136
0.133	0.188
0.25	0.286
0.5	0.408
1	0.597
1.98	0.779
4	0.917
7	0.95
23.0	0.974
30.3	0.956
52.6	0.958
145	0.97
217	0.976

310300
LPE/C18/CO/30C/L

t, h	Mt/Mo
0.25	7.95E-4
0.5	0.00127
1	0.00258
1.5	0.00376
2.5	0.00558
4	0.006
5.5	0.00793
9	0.011
24	0.0199
32	0.0241
50	0.0295
96.2	0.0405
168	0.0529
240	0.0609
384	0.0763
504	0.0877
750	0.107
920	0.116
1204	0.133
1567	0.15
1924	0.166
2399	0.186
2903	0.205
3413	0.22
3911	0.234
4375	0.249
4878	0.268
5459	0.278
6030	0.295
6530	0.308
7062	0.319
7830	0.333
8472	0.346
[illegible]	[illegible]

310600
LPE/C18/CO/60C/L

t, h	Mt/Mo
0.017	0.00268
0.033	0.00447
0.067	0.00707
0.133	0.013
0.25	0.0208
0.5	0.0387
1	0.0602
1.5	0.0743
2.5	0.0936
4	0.117
5.5	0.136
8.5	0.165
24	0.259
32	0.299
55	0.385
81	0.46
150	0.592
240	0.73
337	0.815
488	0.883
721	0.935
1154	0.966
1400	0.949
1584	0.971
1920	0.966
2404	0.983
3030	0.942
3030	0.944

320600
LPE/C18/EN/60C/L

t, h	Mt/Mo
0.017	0.00284
0.033	0.00434
0.067	0.00758
0.133	0.0155
0.25	0.0275
0.5	0.0439
1.5	0.0803
2.5	0.102
4	0.129
5.5	0.148
8	0.175
24	0.286
32	0.329
56	0.437
105	0.58
170	0.701
241	0.762
344	0.798
505	0.831
720	0.852
1086	0.873
1273	0.879
1583	0.872
1945	0.878
1947	0.886
2400	0.892
2400	0.891
2883	0.889
2883	0.805

321600
LPE/C18/.1EN/60C/L

t, h	Mt/Mo
24	8.42E-5
96	2.2E-4
192	2.63E-4
528	2.86E-4
792	2.72E-4
1464	2.79E-4

323600
LPE/C18/.3EN/60C/L

t, h	Mt/Mo
24	4.09E-4
96	7.31E-4
192	7.28E-4
528	7.03E-4
792	7.05E-4
1464	6.57E-4

325600
LPE/C18/.5EN/60C/L(1)

t, h	Mt/Mo
0.017	3.85E-4
0.067	0.00109
0.167	0.00215
0.333	0.00418
1.07	0.0118
2	0.0196
4	0.0264
7	0.0349
23.7	0.0481
30	0.0484
95.8	0.0533
193	0.0445
340	0.0262
533	0.0235
672	0.0212

325602
LPE/C18/.5EN/60C/L(2)

t, h	Mt/Mo
0.167	0.00246
0.333	0.00403
0.667	0.00769
1	0.0106
2	0.0165
4	0.0219
6.75	0.0233
23.8	0.0248

330241
LPE/C18/HP/24C/U

t, h	Mt/Mo
0.067	0.0153
0.133	0.0203
0.25	0.0286
0.5	0.0393
1	0.0559
2	0.0856
4	0.128
8	0.196
27.3	0.467
71.3	0.663
151	0.787
244	0.834
293	0.848
317	0.853
461	0.869
511	0.873
604	0.878
775	0.887
1008	0.894

330301
LPE/C18/HP/30C/U

t, h	Mt/Mo
0.033	0.00727
0.067	0.0108
0.133	0.0169
0.25	0.0248
0.5	0.0382
1	0.0584
1.5	0.0757
2.5	0.107
4	0.153
5.5	0.201
9	0.31
24	0.542
33	0.607
48	0.671
56	0.694
126	0.78
175	0.804
224	0.819
337	0.838
489	0.853
720	0.866
871	0.872
1204	0.882
1536	0.888
1901	0.893
2407	0.898
2905	0.902
3409	0.905
3894	0.908
4517	0.91

330601
LPE/C18/HP/60C/U

t, h	Mt/Mo
0.033	0.0582
0.067	0.0906
0.133	0.139
0.25	0.2
0.5	0.3
1	0.464
1.5	0.626
2.5	0.826
4	0.908
5.5	0.927
9	0.94
24	0.952
33	0.956
55	0.96
97	0.964
104	0.965
175	0.968
242	0.97
338	0.972
537	0.975
720	0.976
919	0.977
1200	0.978
1536	0.98
1564	0.98

340301
LPE/C18/OD/30C/U

0.083	0.00473
0.167	0.0087
0.333	0.0145
0.667	0.0228
1	0.0303
2	0.0484
4	0.0772
7	0.112
23	0.241
31	0.295
96	0.689
103	0.715
144	0.774
199	0.801
267	0.819
360	0.834
456	0.844
696	0.861
1272	0.882
1613	0.889
1942	0.895
2380	0.9
2886	0.905
3507	0.91

340601
LPE/C18/OD/60C/U

t, h	Mt/Mo
0.033	0.0411
0.067	0.0628
0.133	0.0945
0.25	0.136
0.5	0.196
1	0.285
1.5	0.352
2.5	0.463
4	0.595
5.5	0.708
8	0.809
24	0.923
32	0.933
57	0.943
122	0.954
176	0.958
225	0.96
344	0.964
481	0.967
720	0.97
1038	0.972
1302	0.974
1560	0.975
1900	0.977
2405	0.979

370300
LPE/C18/TO/30C/L

t, h	Mt/Mo
0.017	8.81E-4
0.033	8.03E-4
0.067	8.71E-4
0.133	0.00103
0.25	0.00144
0.5	0.00184
1	0.00256
1.5	0.00362
2.5	0.00517
4	0.00763
5.5	0.0092
8	0.0114
25	0.0241
48	0.033
56	0.0359
120	0.0509
168	0.0597
336	0.0816
480	0.0988
702	0.116
872	0.129
1199	0.147
1540	0.169
1969	0.189
2399	0.208
2908	0.23
3408	0.245
3888	0.262
4343	0.279
4830	0.302
5411	0.309
5982	0.328
6482	0.341
7014	0.354
7782	0.376
8425	0.388
8957	0.399

370600
LPE/C18/TO/60C/L

t, h	Mt/Mo
0.017	0.00409
0.033	0.00611
0.067	0.00857
0.133	0.0153
0.25	0.0268
0.5	0.0441
1	0.067
1.5	0.0817
2.5	0.104
4	0.131
5.5	0.153
8	0.181
24	0.296
32	0.339
101	0.563
176	0.72
176	0.72
269	0.837
338	0.876
487	0.918
705	0.94
1106	0.949
1352	0.949
1536	0.944
2021	0.942
2021	0.942

380600
LPE/C18/AQ/60C/L

t, h	Mt/Mo
149	0.00147
216	0.00261
388	0.00707
624	0.0165
866	0.0268
1182	0.0352
1538	0.0522
1968	0.0642
2357	0.0743
2909	0.0880
3480	0.0986
4060	0.106
4705	0.117
5335	0.12

430241
LPE/C18/HP/24C/U

t, h	Mt/Mo
0.033	0.0148
0.067	0.0258
0.133	0.0411
0.25	0.0628
0.5	0.108
1	0.202
2	0.342
4	0.477
20	0.693
28	0.732
92	0.817
146	0.838
196	0.851
289	0.861
460	0.873
693	0.865

530301
LPE/C18/HP/30C/U

t, h	Mt/Mo
0.017	0.0834
0.033	0.143
0.083	0.184
0.167	0.279
0.333	0.385
0.5	0.458
0.75	0.542
1	0.612
1.25	0.678
1.75	0.772
2.75	0.867
4.25	0.925
5.75	0.947
7.75	0.96
24.3	0.979
31.8	0.981
96	0.987
145	0.988
199	0.989
265	0.99
439	0.991
534	0.991
652	0.991
663	0.994

540301
LPE/C18/OD/30C/U

t, h	Mt/Mo
0.167	0.129
0.333	0.185
0.667	0.264
1	0.319
2	0.426
4	0.561
8	0.714
24	0.94
48	0.991
79.5	0.997
168	0.999
217	0.999
271	0.999
389	1

540601
LPE/C18/OD/60C/U

t, h	Mt/Mo
0.167	0.169
0.333	0.278
0.667	0.404
1	0.493
1.5	0.601
2.5	0.734
4	0.864
6	0.937
8	0.971
23	0.994
31.5	0.995
120	0.995
169	0.996
217	0.996
31	0.996

640301
LPE/C18/0D/30C/U

t, h	Mt/Mo
0.012	0.109
0.017	0.128
0.025	0.155
0.033	0.18
0.05	0.219
0.067	0.254
0.083	0.285
0.104	0.317
0.133	0.361
0.167	0.405
0.25	0.522
0.337	0.599
0.504	0.708
0.667	0.784
1	0.875
1.5	0.934
2	0.955
3	0.968
4.5	0.972
6	0.975
8	0.976
25.3	0.981

640601
LPE/C18/0D/60C/U

t, h	Mt/Mo
0.033	0.376
0.083	0.582
0.167	0.772
0.333	0.923
0.667	0.981
1	0.99
1.5	0.992
2	0.992
3	0.993
4.5	0.993
7	0.994
24	0.995
48	0.995
103	0.996
199	0.997

710301
BPE/C18/CO/30C/U

t, h	Mt/Mo
0.033	0.0115
0.067	0.0216
0.133	0.0323
0.25	0.044
0.5	0.0581
1	0.0749
1.5	0.0895
2.5	0.109
4	0.131
5.5	0.15
8	0.174
24	0.258
48	0.341
81.2	0.425
144	0.532
241	0.624
389	0.708
582	0.769
865	0.817
1181	0.849
1543	0.873
1921	0.891
2406	0.908
2885	0.922
3770	0.938
4284	0.95
4854	0.96
5407	0.971

710601
BPE/C18/CO/60C/U

t, h	Mt/Mo
0.017	0.0332
0.033	0.0641
0.067	0.093
0.133	0.134
0.25	0.188
0.5	0.267
1	0.368
1.5	0.447
3	0.602
5.25	0.745
7	0.819
24	0.945
32	0.958
55	0.97
124	0.98
364	0.989
1157	0.999

720301
BPE/C18/EN/30C/U

t, h	Mt/Mo
0.033	0.00813
0.067	0.0106
0.133	0.0145
0.25	0.0199
0.5	0.0286
1	0.0419
1.5	0.0519
2.5	0.0694
4	0.0903
5.5	0.108
8	0.132
24.2	0.244
48.3	0.356
120	0.556
216	0.689
385	0.789
555	0.838
866	0.881
1181	0.904
1537	0.919
2022	0.932
2401	0.939
2881	0.945
3339	0.95

720601
BPE/C18/EN/60C/U

t, h	Mt/Mo
0.017	0.0527
0.033	0.0743
0.067	0.104
0.133	0.146
0.25	0.198
0.5	0.286
1	0.411
2	0.582
4	0.779
6	0.877
7.5	0.917
24	0.99
98.3	0.998
509	0.999
1277	0.999

730301
BPE/C18/HP/30C/U

t, h	Mt/Mo
0.033	0.0457
0.067	0.0692
0.133	0.106
0.25	0.157
0.5	0.243
1	0.376
1.5	0.499
2.5	0.72
4	0.862
5.5	0.912
8	0.942
24	0.974
32	0.977
48	0.98
119	0.986
215	0.988
383	0.989
628	0.99

730601
BPE/C18/HP/60C/U

t, h	Mt/Mo
0.017	0.16
0.033	0.229
0.067	0.336
0.133	0.484
0.25	0.693
0.5	0.932
1	0.996
1.5	0.999
2.5	0.999
4.5	1
23.5	1
95.8	1
267	1

770301
BPE/C18/TO/30C/U

t, h	Mt/Mo
0.033	0.0127
0.067	0.0224
0.133	0.0323
0.25	0.0434
0.5	0.0571
1	0.0738
1.5	0.0883
2.5	0.108
4	0.13
5.5	0.15
8	0.174
24.1	0.264
48.2	0.353
76.5	0.429
96.4	0.474
216	0.626
386	0.724
605	0.785
870	0.824
1177	0.85
1536	0.87
1950	0.885
2406	0.898
2888	0.908
3368	0.917
3701	0.932

770601
BPE/C18/TO/60C/U

t, h	Mt/Mo
0.017	0.0448
0.033	0.0731
0.067	0.109
0.133	0.154
0.25	0.208
0.5	0.286
1.02	0.397
1.5	0.475
2.5	0.592
4	0.716
5.5	0.793
7.5	0.856
24	0.934
31.5	0.946
71.3	0.96
169	0.972
748	0.984
1537	0.997

830301
BPE/C18/HP/30C/U

t, h	Mt/Mo
0.006	0.0452
0.008	0.057
0.017	0.0859
0.033	0.129
0.067	0.187
0.133	0.274
0.25	0.388
0.5	0.582
1	0.814
1.5	0.901
2.5	0.955
4	0.976
5.67	0.982
7	0.984
23.8	0.99
31.3	0.991
48	0.992
74.9	0.993
173	0.994

840301
BPE/C18/OD/30C/U1

t, h	Mt/Mo
0.004	0.0225
0.008	0.0402
0.021	0.0587
0.033	0.0737
0.05	0.0905
0.083	0.117
0.117	0.14
0.183	0.176
0.233	0.197
0.35	0.24
0.5	0.279
0.733	0.345
0.983	0.4
1.48	0.484
1.98	0.55
2.98	0.649
3.98	0.721
5.98	0.82
8.98	0.904
23.8	0.987
32	0.991
48.2	0.993
56.4	0.993
72.3	0.994
80.3	0.994
168	0.995
173	0.995

840302
BPE/C18/OD/30C/U2

t, h	Mt/Mo
0.011	0.037
0.019	0.0466
0.025	0.0546
0.035	0.0656
0.053	0.0774
0.067	0.089
0.1	0.11
0.133	0.126
0.183	0.147
0.25	0.172
0.333	0.198
0.483	0.238
0.736	0.294
0.985	0.339
1.49	0.415
1.98	0.477
2.98	0.577
4.53	0.694
5.98	0.771
8.22	0.852
23.9	0.981
32.3	0.987
47.6	0.989
56.3	0.99
73.5	0.99
73.5	0.99

840601
BPE/C18/OD/60C/U

t, h	Mt/Mo
0.005	0.0654
0.011	0.104
0.017	0.143
0.025	0.166
0.033	0.198
0.05	0.218
0.067	0.248
0.1	0.305
0.133	0.35
0.167	0.391
0.25	0.476
0.333	0.544
0.5	0.652
0.75	0.77
1	0.848
1.5	0.932
2	0.969
3	0.992
5	0.998
8	0.998
24	0.999
32	0.999
48	0.999
56	0.999
144	0.999
150	0.999

920300
BPE/C18/EH/30C/L

t, h	Mt/Mo
0.067	0.0086
0.133	0.0166
0.25	0.0196
0.5	0.0317
1	0.0479
1.97	0.0679
4	0.094
6.25	0.118
24	0.231
30.8	0.271
55.8	0.391
96.3	0.511
144	0.555
193	0.633
264	0.7
316	0.713
361	0.728
433	0.767
481	0.765
601	0.791
701	0.823

920600
BPE/C18/EH/60C/L

t, h	Mt/Mo
0.017	0.053
0.033	0.0781
0.067	0.0955
0.133	0.127
0.25	0.177
0.5	0.273
1	0.404
1.5	0.504
2.5	0.641
4	0.802
5.5	0.884
8.1	0.959
23.7	1
31.5	1.04
49.9	0.995
78.7	0.996
171	0.988
384	0.987
580	0.981
841	0.974
1014	0.939
1014	0.947

925300
BPE/C18/.5EN/30C/L

t, h	Mt/Mo
2.5	0.00399
4	0.00655
5.78	0.0102
8	0.0101
23.6	0.0151
31.5	0.0158
48.1	0.0163
55.7	0.0158
122	0.0179
216	0.0172
216	0.0167
384	0.0168
486	0.0172
486	0.0196

925600
BPE/C18/.5EN/60C/L

t, h	Mt/Mo
0.133	0.00479
0.25	0.00762
0.5	0.0141
1	0.0263
1.5	0.0359
2.5	0.0501
4	0.0582
5.5	0.0626
8	0.0637
23.9	0.0681
31.8	0.0675
97.7	0.0659
170	0.0673
360	0.0669
509	0.0699
509	0.0745

995300
BPE/C18/.95EN/30C/L

t, h	Mt/Mo
1	0.0254
1.5	0.0469
2.02	0.0478
3.28	0.0668
5.15	0.0957
7.5	0.121
23.7	0.213
30.1	0.263
48.1	0.335
53.5	0.348
121	0.506
170	0.584
289	0.698
389	0.696
457	0.746
553	0.747
796	0.782
961	0.788
965	0.819

995600
BPE/C18/.95EN/60C/L

t, h	Mt/Mo
0.067	0.0586
0.133	0.0966
0.25	0.145
0.5	0.229
1	0.37
2	0.526
4	0.747
5.30	0.816
7.15	0.866
24.1	0.974
31.1	0.993
48.4	0.928
71.9	0.934
145	0.977
197	0.984

940301
BPE/C18/OD/30C/U

t, h	Mt/Mo
0.017	0.0134
0.033	0.0198
0.067	0.0293
0.117	0.0395
0.183	0.0508
0.25	0.0602
0.5	0.0883
0.75	0.111
1	0.13
1.5	0.162
2	0.19
2.5	0.214
4	0.277
5.5	0.329
8	0.404
24	0.706
33.7	0.86
48	0.941
56.2	0.956
72.3	0.966
98.6	0.972
172	0.978

940601
BPE/C18/OD/60C/U

t, h	Mt/Mo
0.017	0.0766
0.033	0.11
0.067	0.164
0.117	0.222
0.183	0.283
0.25	0.334
0.5	0.48
0.75	0.598
1	0.7
1.5	0.844
2	0.927
2.5	0.967
4	0.995
5.75	0.997
8	0.998
23.9	0.998
32.1	0.998
48.2	0.998
108	0.998

950300
BPE/C18/ON/30C/L

t, h	Mt/Mo
0.117	0.00905
0.183	0.0151
0.3	0.0212
0.5	0.0282
0.833	0.0427
1.5	0.0616
2.5	0.0826
4.25	0.107
7.03	0.151
23.8	0.283
30.9	0.325
48.1	0.425
123	0.658
217	0.788
386	0.881
626	0.913
889	0.927
1202	0.937
1494	0.895
2019	0.947

950600
BPE/C18/ON/60C/L

t, h	Mt/Mo
0.017	0.0557
0.033	0.0717
0.067	0.0942
0.133	0.134
0.25	0.193
0.5	0.293
1	0.444
2	0.64
4	0.85
6.03	0.932
7.38	0.957
24	0.982
30.7	0.976
75.5	0.98
149	0.992

960300
BPE/C18/TB/30C/L

t, h	Mt/Mo
0.133	0.0157
0.25	0.0245
0.5	0.0264
1	0.0456
1.98	0.0695
4	0.0912
6	0.117
7.42	0.125
23.9	0.218
31.5	0.273
57.5	0.346
96.1	0.466
145	0.544
196	0.599
264	0.667
312	0.694
361	0.725
432	0.752
484	0.77
529	0.787
601	0.813
649	0.811
769	0.832
989	0.854

960600
BPE/C18/TB/60C/L

t, h	Mt/Mo
0.017	0.0287
0.033	0.0398
0.067	0.0503
0.117	0.0703
0.183	0.103
0.25	0.11
0.5	0.196
0.75	0.265
1	0.314
1.5	0.401
2	0.47
2.5	0.532
3.5	0.642
5.02	0.761
7	0.847
8.83	0.918
24.9	0.986
32.7	0.992
55.3	0.978
80.5	0.983
151	0.97
389	0.988

980600
BPE/C18/AQ/60C/L

t, h	Mt/Mo
3292	0.00434
4036	0.00727
4731	0.0112
5593	0.0218
6312	0.0311
7057	0.045
7540	0.059

990400
BPE/C18/HB/40C/L

t, h	Mt/Mo
0.5	0.0522
1	0.0783
1.97	0.103
4	0.172
5.53	0.235
6.78	0.254
24.3	0.502
30.5	0.561
54	0.664
75.7	0.722
145	0.805
193	0.846
313	0.848
409	0.867
529	0.846
724	0.869

990600
BPE/C18/HB/60C/L

t, h	Mt/Mo
0.017	0.0273
0.033	0.0238
0.067	0.074
0.133	0.108
0.25	0.15
0.5	0.246
1	0.364
2	0.531
3	0.646
20.5	0.957
24.1	0.976
27	0.974
44.8	0.987
141	0.984
358	0.979

1120600
LPE/C18/EN/60C/L

t, h	Mt/Mo
0.017	0.00278
0.033	0.00381
0.067	0.00635
0.133	0.00849
0.25	0.0126
0.5	0.022
1	0.0326
1.5	0.0397
2.5	0.0506
4	0.0637
5.5	0.0732
8	0.087
23.7	0.141
31.3	0.16
95.9	0.265
192	0.356
364	0.486
605	0.595
990	0.69
1200	0.724
1612	0.803
1613	0.802
1872	0.822
2094	0.775
2862	0.746
3652	0.869
4999	0.868
5715	0.907

1130301
LPE/C18/HP/30C/U

t, h	Mt/Mo
0.017	0.0019
0.033	0.00304
0.067	0.00489
0.133	0.0076
0.25	0.0111
0.5	0.017
1	0.0259
1.5	0.033
2.5	0.0451
4.02	0.0607
5.5	0.0739
8.42	0.0939
24.1	0.187
32.4	0.227
96.1	0.45
149	0.553
200	0.618
367	0.736
602	0.797
870	0.838
1178	0.861
1537	0.876
1970	0.887
2387	0.893
2882	0.9
3294	0.904
3733	0.908
4207	0.911
4688	0.913
5211	0.915
5694	0.917
6173	0.919
6676	0.92

1520600
BPE/C32/EN/60C/L

t, h	Mt/Mo
0.017	0.0109
0.033	0.0154
0.067	0.0201
0.133	0.0287
0.25	0.0441
0.5	0.0693
1	0.104
1.5	0.13
2.5	0.171
4	0.218
5.5	0.254
8	0.303
24	0.404
55.3	0.625
121	0.693
289	0.725
384	0.74
676	0.749
677	0.75
865	0.75
1183	0.751
1538	0.757
1997	0.76
2191	0.755

1530300
BPE/C32/HP/30C/L

t, h	Mt/Mo
0.017	0.00234
0.033	0.00357
0.067	0.00516
0.133	0.00814
0.25	0.0121
0.5	0.0198
1	0.0322
1.98	0.0528
4	0.0935
5.72	0.121
6.82	0.136
23.9	0.267
30.4	0.307
47.6	0.379
77.2	0.434
145	0.525
241	0.632
508	0.715
697	0.741
894	0.755
1153	0.759
1489	0.751
1732	0.783

1530601
BPE/C32/HP/60C/U

t, h	Mt/Mo
0.017	0.0625
0.033	0.097
0.067	0.154
0.133	0.239
0.25	0.348
0.5	0.558
1	0.803
1.5	0.888
2.5	0.94
4	0.959
5.5	0.965
8	0.97
24	0.98
47.8	0.984
96.1	0.987
200	0.99
391	0.992
606	0.992
889	0.993
1176	0.994
1512	0.994
1950	0.994
2043	0.994

1610300
BPE/C32/CO/30C/L

t, h	Mt/Mo
0.017	9.35E-4
0.033	0.00106
0.067	0.00164
0.133	0.00226
0.2	0.0028
0.25	0.00342
0.5	0.00488
0.75	0.00654
1	0.00789
1.5	0.01
2	0.0118
2.5	0.0135
4	0.0175
5.5	0.0209
9.07	0.0271
24.7	0.0437
32.5	0.0504
47.8	0.0604
80	0.0779
146	0.103
221	0.123
386	0.155
577	0.185
843	0.219
1154	0.25
1519	0.29
1902	0.306
2414	0.339
2887	0.364
3369	0.385
3914	0.405
4375	0.421
4850	0.436
5379	0.45
5885	0.462
6433	0.473
6942	0.482

1610600
BPE/C32/CO/60C/L

t, h	Mt/Mo
0.017	0.0132
0.033	0.0194
0.067	0.0282
0.133	0.0381
0.2	0.0529
0.25	0.0618
0.5	0.11
0.75	0.154
1	0.176
1.5	0.242
2	0.29
2.5	0.33
4	0.433
5.5	0.508
7.83	0.595
24.3	0.811
31.8	0.85
97.8	0.912
194	0.952
360	0.948
602	0.95
844	0.947
1327	0.958

1620300
BPE/C32/EN/30C/L

t, h	Mt/Mo
0.017	2.41E-4
0.033	3.18E-4
0.067	4.95E-4
0.133	8.26E-4
0.25	0.00132
0.5	0.00217
1	0.00347
1.5	0.00469
2.5	0.00649
4.07	0.0093
5.5	0.0114
7.8	0.0146
23.7	0.0277
31.8	0.0334
55.8	0.0437
104	0.059
264	0.0881
432	0.108
654	0.126
1422	0.145
2211	0.166
3559	0.166
4638	0.152
5310	0.145
6389	0.156

1620600
BPE/C32/EN/60C/L

t, h	Mt/Mo
0.017	0.02
0.033	0.0263
0.067	0.0341
0.133	0.0515
0.25	0.0815
0.5	0.138
1	0.217
1.5	0.275
2.5	0.363
4	0.462
8.05	0.622
24.3	0.803
31.9	0.813
55.9	0.837
79.7	0.835
151	0.848
245	0.849
384	0.844
486	0.854
700	0.851
988	0.856
1248	0.858
1470	0.844
1710	0.847
1710	0.857

1625600
BPE/C32/.5EN/60C/L

t, h	Mt/Mo
0.017	2.55E-4
0.033	3.78E-4
0.067	5.06E-4
0.133	7.51E-4
0.25	0.00116
0.5	0.00197
1	0.00323
1.5	0.00421
2.5	0.00561
4	0.00747
5.5	0.00847
7.87	0.00961
23.7	0.0114
31.9	0.0121
55.9	0.0123
79.5	0.0122
240	0.0125
408	0.0109
630	0.0103
2697	0.0107

1695300
BPE/C32/.95EN/30C/L

t, h	Mt/Mo
0.033	2.08E-4
0.067	3.26E-4
0.133	5.08E-4
0.25	8.6E-4
0.5	0.00137
1	0.00231
2.05	0.00391
4	0.00635
5.37	0.00787
23.7	0.0203
29.5	0.0238
48.5	0.0319
77.2	0.0403
149	0.0552
316	0.0754
504	0.0923
673	0.0991
841	0.108
1177	0.117
1441	0.116
1733	0.123
1901	0.137

1695600
BPE/C32/.95EN/60C/L

t, h	Mt/Mo
0.017	0.0123
0.033	0.0191
0.067	0.029
0.133	0.0459
0.25	0.0738
0.5	0.122
1	0.193
2.07	0.293
4	0.409
7	0.519
24.1	0.7
30.2	0.71
53.5	0.738
120	0.741
172	0.807

1630301
BPE/C32/HP/30C/U

t, h	Mt/Mo
0.017	0.00788
0.033	0.012
0.067	0.0178
0.133	0.0272
0.2	0.0361
0.25	0.0422
0.5	0.0742
0.75	0.104
1	0.128
1.5	0.168
2	0.198
2.5	0.223
4	0.285
5.5	0.335
8	0.397
23.9	0.585
32.1	0.627
47.9	0.674
79.9	0.721
146	0.763
246	0.789
385	0.809
584	0.825
872	0.84
1184	0.85
1540	0.858
1922	0.865
2407	0.873
2941	0.879
3415	0.883
3921	0.887
4615	0.891

1630601
BPE/C32/HP/60C/U

t, h	Mt/Mo
0.017	0.16
0.033	0.251
0.067	0.401
0.133	0.662
0.2	0.791
0.25	0.841
0.5	0.916
0.75	0.934
1	0.942
1.5	0.952
2	0.956
2.5	0.959
4	0.965
5.5	0.969
8	0.972
23.8	0.978
32	0.98
48.1	0.982
55.8	0.982
123	0.985
222	0.988
342	0.988
391	0.989
628	0.99
870	0.99
1178	0.991
1565	0.991
1661	0.991

1650300
BPE/C32/ON/30C/L

t, h	Mt/Mo
0.017	1.7E-4
0.033	2.52E-4
0.067	3.79E-4
0.117	6.08E-4
0.183	9.4E-4
0.3	0.00136
0.5	0.00207
0.833	0.00309
1.5	0.005
2.5	0.00748
4.25	0.0112
7	0.0164
24	0.0304
31.1	0.0464
51.4	0.0645
98.9	0.0969
200	0.151
362	0.23
602	0.284
865	0.324
1178	0.364
1470	0.395
1897	0.428
2401	0.459
2906	0.483
3488	0.505
4081	0.525
4729	0.543
5435	0.558
6169	0.574
6264	0.581

1650600
BPE/C32/ON/60C/L

t, h	Mt/Mo
0.017	0.0296
0.033	0.0371
0.067	0.0471
0.133	0.0654
0.25	0.103
0.5	0.169
1	0.262
2	0.387
4	0.572
6	0.675
7.5	0.744
23.7	0.874
31.3	0.881
48.1	0.893
99.5	0.924
145	0.919
217	0.936

1660300
BPE/C32/TB/30C/L

t, h	Mt/Mo
0.017	3.21E-4
0.033	5.33E-4
0.067	9.16E-4
0.117	0.0014
0.183	0.00204
0.3	0.00297
0.5	0.0044
0.833	0.00646
1.5	0.0101
2.5	0.0145
3.75	0.0199
5.3	0.0252
7.25	0.0308
23	0.0618
31.3	0.0746
51.9	0.0976
79.3	0.123
144	0.168
220	0.208
385	0.277
579	0.342
871	0.405
1201	0.464
1538	0.514
1925	0.563
2401	0.613
2931	0.659
3412	0.701

1660600
BPE/C32/TB/60C/L

t, h	Mt/Mo
0.017	0.019
0.033	0.027
0.067	0.0387
0.133	0.0558
0.25	0.0814
0.5	0.13
1	0.199
2	0.291
4	0.426
6	0.52
7.55	0.581
23.9	0.805
30.8	0.832
48.3	0.865
72	0.877
169	0.906
240	0.905
340	0.915
505	0.921
673	0.916
961	0.932

1670300
BPE/C32/TO/30C/L

t, h	Mt/Mo
0.017	2.7E-4
0.033	4.17E-4
0.067	6.34E-4
0.133	9.36E-4
0.2	0.00128
0.25	0.00148
0.5	0.00243
0.75	0.00337
1	0.00424
1.5	0.00569
2	0.00703
2.5	0.00825
4	0.0115
5.5	0.0142
8	0.0184
23.8	0.0361
47.8	0.0552
79.6	0.0749
146	0.102
217	0.123
392	0.16
577	0.197
865	0.239
1157	0.271
1518	0.302
1897	0.343
2412	0.358
2983	0.389
3483	0.408
4015	0.425
4514	0.44
5045	0.452
5522	0.477
6027	0.47
[illegible]	[illegible]

1670600
BPE/C32/TO/60C/L

t, h	Mt/Mo
0.017	0.0106
0.033	0.0157
0.067	0.0231
0.133	0.0417
0.2	0.0609
0.25	0.0735
0.5	0.136
0.75	0.181
1	0.218
1.5	0.281
2	0.333
2.5	0.379
4	0.49
5.5	0.574
8	0.668
23.9	0.846
31.9	0.874
48	0.896
55.5	0.905
122	0.919
218	0.937
385	0.947
629	0.948
866	0.951
1155	0.948
1688	0.954

1680600
BPE/C32/AQ/60C/L

t, h	Mt/Mo
1	1.81E-4
2	2.55E-4
4	3.42E-4
8	4.11E-4
24	5.06E-4
48.4	6.83E-4
122	7.84E-4
397	0.00132
725	0.00176
1346	0.00225
1925	0.00275
2597	0.00303
3269	0.00377
4012	0.00476
4708	0.00563
5593	0.00793
6289	0.0102
7034	0.0125
7538	0.0175

1690400
BPE/C32/HB/40C/L

t, h	Mt/Mo
0.017	8.12E-4
0.033	0.00231
0.067	0.00255
0.15	0.00614
0.25	0.00954
0.5	0.016
1	0.025
1.97	0.0378
4	0.0562
6	0.0705
7.42	0.0783
24.3	0.14
30.3	0.158
51.8	0.205
121	0.307
169	0.36
221	0.409
289	0.458
385	0.515
556	0.586
864	0.651
1009	0.674
1301	0.698
1468	0.71
1732	0.725
1993	0.736
2329	0.751
2405	0.753

1690600
BPE/C32/HB/60C/L

t, h	Mt/Mo
0.017	0.0298
0.033	0.0328
0.067	0.0497
0.133	0.0662
0.25	0.0991
0.5	0.167
1	0.248
1.95	0.36
4	0.516
6	0.617
23.7	0.856
30.5	0.882
51.6	0.895
72.4	0.919
169	0.936
313	0.943
481	0.947
508	0.954

1910300
LPE/C32/CO/30C/L

t, h	Mt/Mo
0.017	1.77E-4
0.033	1.52E-4
0.067	1.94E-4
0.133	2.97E-4
0.25	3.26E-4
0.5	6.85E-4
1	0.00105
1.5	0.00143
2.5	0.00197
4	0.00273
5.5	0.00340
8	0.00459
23.7	0.00968
31.2	0.0119
47.9	0.0155
79.6	0.0207
145	0.0272
218	0.0324
385	0.0421
553	0.0498
840	0.0584
1154	0.0643
1518	0.071
1908	0.0762
2479	0.084
2979	0.0898
3511	0.0943
4010	0.0996
4443	0.103
4925	0.107
5618	0.112

1910600
LPE/C32/CO/60C/L

t, h	Mt/Mo
0.017	0.00139
0.033	0.00263
0.067	0.00375
0.133	0.00665
0.2	0.00932
0.25	0.0116
0.5	0.0222
0.75	0.0306
1	0.0375
1.5	0.0484
2	0.0562
2.5	0.0617
4	0.0762
5.5	0.0866
8	0.101
24	0.154
32	0.176
48.3	0.205
55.6	0.22
121	0.301
216	0.386
385	0.496
601	0.596
840	0.657
1177	0.707
1519	0.73
2053	0.768
2527	0.782
3003	0.789
3511	0.801

1920300
LPE/C32/EN/30C/L

t, h	Mt/Mo
0.067	1.75E-4
0.133	2.94E-4
0.25	4.02E-4
0.5	7.69E-4
1	0.00122
2	0.00213
4	0.00349
6	0.0047
7.63	0.0056
24	0.0112
31	0.0123
125	0.0223
221	0.0262
385	0.0301
556	0.0325
697	0.0331
822	0.035
1036	0.0349
1204	0.0355
1371	0.0353
1633	0.036
1853	0.0362
1897	0.0361
2557	0.0375
3318	0.0383
3318	0.0385

1920600
LPE/C32/EN/60C/L

t, h	Mt/Mo
0.017	0.00324
0.033	0.00476
0.067	0.00705
0.133	0.013
0.25	0.0219
0.5	0.0365
1	0.0558
2	0.0741
4	0.0965
6	0.112
7.75	0.125
24	0.188
30.5	0.213
48	0.245
72	0.287
149	0.381
245	0.452
409	0.544
580	0.576
721	0.59
846	0.584
1061	0.6
1228	0.548
1395	0.611
1657	0.593
1877	0.609
2140	0.583
2581	0.623
3365	0.623
3365	0.627

1925600
LPE/C32/.5EN/60C/L

t, h	Mt/Mo
0.5	1.59E-4
1	3.51E-4
1.5	3.92E-4
2.5	5.28E-4
4.1	7.02E-4
5.5	8.64E-4
7.85	1.0E-3
23.7	0.00135
31.9	0.00147
55.9	0.00167
216	0.00262
384	0.00309
1110	0.00396
1878	0.00462

1930301
LPE/C32/HP/30C/U

t, h	Mt/Mo
0.017	0.00242
0.033	0.00398
0.067	0.00656
0.133	0.0102
0.25	0.0149
0.5	0.022
1	0.0323
2	0.0489
4	0.0829
6	0.115
7.5	0.134
24.1	0.245
31.5	0.274
54.5	0.332
79	0.372
172	0.455
223	0.483
313	0.519
387	0.541
416	0.549
583	0.58
747	0.602
917	0.618
1057	0.628
1326	0.638
1540	0.649
1708	0.659
1875	0.668
2137	0.678
2357	0.686
2620	0.694
3002	0.704
3265	0.712
4243	0.72
4487	0.73
4823	0.734

1930601
LPE/C32/HP/60C/U

t, h	Mt/Mo
0.017	0.0282
0.033	0.0414
0.067	0.0611
0.133	0.0908
0.25	0.132
0.5	0.205
1	0.332
2	0.53
4	0.69
6	0.75
8	0.782
23.5	0.858
31.2	0.872
96	0.909
152	0.924
292	0.936
433	0.941
701	0.947
866	0.95
1036	0.952
1156	0.954

1950300
LPE/C32/ON/30C/L

t, h	Mt/Mo
0.183	2.42E-4
0.3	4.64E-4
0.5	7.1E-4
0.833	0.00119
1.5	0.00197
2.5	0.00301
4.25	0.00438
7	0.00634
24	0.0137
31	0.0159
49.1	0.0207
79	0.027
148	0.0438
241	0.0517
384	0.0616
576	0.0716
868	0.0845
1182	0.0959
1541	0.107
1944	0.116
2400	0.125
2932	0.134
3460	0.14
4079	0.15
4732	0.156
5430	0.166
6101	0.171

1950600
LPE/C32/ON/60C/L

t, h	Mt/Mo
0.017	0.00321
0.033	0.0046
0.067	0.00718
0.133	0.0116
0.25	0.0195
0.5	0.0317
1.03	0.05
1.97	0.0701
4	0.0985
6	0.119
6.88	0.128
24.3	0.222
49.4	0.345
121	0.491
168	0.543
221	0.591
292	0.637
457	0.686
624	0.718
817	0.756
961	0.764
1129	0.746
1345	0.744
1542	0.787
1830	0.795
2185	0.789
2669	0.804

1970300
LPE/C32/TO/30C/L

t, h	Mt/Mo
0.017	2.14E-4
0.033	1.53E-4
0.067	3.99E-4
0.133	4.19E-4
0.2	5.64E-4
0.25	5.98E-4
0.5	8.6E-4
0.75	0.00126
1	0.00153
1.5	0.00221
2.02	0.00263
2.5	0.00321
4	0.00448
5.5	0.00577
8.13	0.00798
23.9	0.017
32.1	0.0196
48.3	0.0235
79.8	0.0291
146	0.0372
224	0.0433
389	0.0547
576	0.0588
844	0.0676
1160	0.0739
1537	0.0803
1904	0.0845
2413	0.0925
2887	0.0979
3363	0.102
3870	0.113
4346	0.111
4879	0.114
5354	0.118
5820	0.121

1970600
LPE/C32/TO/60C/L

t, h	Mt/Mo
0.017	0.00239
0.033	0.00414
0.067	0.0063
0.133	0.0112
0.2	0.0147
0.25	0.0185
0.5	0.0315
0.75	0.0405
1.5	0.059
2	0.0672
2.5	0.073
4	0.0891
5.5	0.0993
8	0.116
24.3	0.174
32	0.194
47.8	0.226
55.8	0.242
122	0.332
217	0.427
385	0.561
625	0.63
840	0.68
1153	0.713
1513	0.736
1880	0.735
2285	0.762
2558	0.781
3031	0.794
3513	0.8
4058	0.811
4543	0.816
4543	0.819

1980600
LPE/C32/AQ/60C/L

t, h	Mt/Mo
5	3.25E-6
23.3	1.04E-4
119	2.21E-4
316	7.08E-4
456	0.00102
623	0.0016
816	0.00212
1205	0.00418
1611	0.00649
1775	0.00782
2111	0.0104
2495	0.0143
2783	0.0166
3119	0.0197
3627	0.0241
4034	0.0272
4703	0.0314

2010300
LPE/BHT/CO/30C/L

t, h	Mt/Mo
0.067	2.85E-4
0.117	4.27E-4
0.183	3.95E-4
0.25	5.21E-4
0.5	9.33E-4
0.75	1.0E-3
1	0.00143
1.5	0.00184
2	0.00245
2.5	0.00286
4.03	0.00386
5.5	0.00526
8	0.00696
24	0.0168
32	0.021
48.4	0.0278
56.2	0.0308
120	0.0528
192	0.0662
364	0.0891
605	0.115
841	0.135
1158	0.156
1547	0.176
1886	0.194
2331	0.213
2858	0.234

2010600
LPE/BHT/CO/60C/L

t, h	Mt/Mo
0.017	6.86E-4
0.033	0.00111
0.067	0.00148
0.117	0.00269
0.183	0.00421
0.25	0.0058
0.5	0.0118
0.75	0.0181
1	0.0224
1.5	0.0305
2	0.0371
2.5	0.0427
4	0.057
5.58	0.0688
8	0.0825
24	0.145
30.9	0.166
47.8	0.208
56.8	0.226
121	0.325
224	0.422
394	0.503
632	0.538
869	0.586
1229	0.584
1469	0.588
1742	0.595
2141	0.601
2574	0.598

2020300
LPE/BHT/EN/30C/L

t, h	Mt/Mo
0.017	3.3E-4
0.033	4.36E-4
0.067	5.25E-4
0.133	7.05E-4
0.25	8.6E-4
0.5	0.00126
1	0.00179
1.5	0.00222
2.5	0.00347
4	0.00462
5.5	0.00592
7.95	0.00767
23.6	0.0156
31.5	0.0187
100	0.0365
192	0.0519
360	0.0708
915	0.107
1495	0.129
1755	0.137
2197	0.151
3027	0.185
3027	0.188

2020600
LPE/BHT/EN/60C/L

t, h	Mt/Mo
0.017	0.00109
0.033	0.00145
0.067	0.00217
0.133	0.00279
0.25	0.00524
0.5	0.00925
1	0.0168
2	0.0266
4	0.0421
6	0.0505
7.5	0.0601
23.8	0.111
31.2	0.126
53.5	0.166
127	0.24
220	0.297
389	0.359
460	0.394
733	0.444
1060	0.455
1705	0.493
1705	0.495

2030301
LPE/BHT/HP/30C/U

t, h	Mt/Mo
0.017	0.00372
0.033	0.00676
0.067	0.0124
0.133	0.0207
0.2	0.027
0.25	0.0314
0.5	0.0495
0.783	0.0677
1	0.081
1.5	0.111
2.02	0.141
2.5	0.17
4	0.269
5.5	0.378
8	0.489
24	0.595
32	0.602
48	0.607
56	0.611
144	0.614
217	0.615
384	0.617
580	0.618
893	0.619

2030601
LPE/BHT/HP/60C/U1

t, h	Mt/Mo
0.017	0.0201
0.033	0.0322
0.067	0.0488
0.133	0.0754
0.2	0.0968
0.25	0.111
0.5	0.177
0.75	0.24
1	0.304
1.5	0.431
2	0.504
2.5	0.541
4.05	0.58
5.5	0.589
9	0.595
23.8	0.6
32	0.6
47.9	0.601
96	0.603
168	0.604
218	0.605
390	0.606
606	0.608
866	0.609
918	0.61

2030602
LPE/BHT/HP/60C/U2

t, h	Mt/Mo
0.017	0.0103
0.033	0.0153
0.067	0.0263
0.133	0.0463
0.25	0.0809
0.5	0.149
1	0.286
1.5	0.411
2.25	0.499
3.5	0.543
5.25	0.558
7.75	0.565
24.6	0.572
37.5	0.574
101	0.577

2070300
LPE/BHT/TO/30C/L

t, h	Mt/Mo
0.017	3.09E-4
0.033	3.71E-4
0.067	4.7E-4
0.117	4.78E-4
0.183	5.17E-4
0.25	7.3E-4
0.5	7.89E-4
0.75	0.0012
1	0.00139
1.5	0.00164
2	0.00202
2.5	0.00243
4	0.00366
5.5	0.00461
8	0.00615
24	0.0148
32	0.0183
48.5	0.0246
76.3	0.0332
128	0.0469
221	0.0655
386	0.0943
631	0.122
899	0.151
1238	0.179
1566	0.205
1971	0.23
2214	0.245

2070600
LPE/BHT/TO/60C/L

t, h	Mt/Mo
0.017	7.13E-4
0.033	0.00102
0.067	0.00169
0.117	0.00229
0.183	0.00368
0.25	0.0046
0.5	0.00976
0.75	0.0143
1	0.0179
1.5	0.0244
2	0.0305
2.52	0.0354
4	0.0487
5.57	0.0605
8	0.0761
23.9	0.145
31.9	0.172
47.9	0.214
101	0.311
152	0.375
217	0.434
389	0.554
584	0.536
923	0.575
1262	0.59
1590	0.597
1995	0.602
2094	0.607

2130601
LPE/BHT/HP/60C/U

t, h	Mt/Mo
0.017	0.0925
0.033	0.139
0.067	0.212
0.133	0.335
0.25	0.531
0.5	0.648
1	0.666
2	0.668
4.5	0.669
7	0.67
24.3	0.671

2210300
LPE/BHT/CO/30C/L

t, h	Mt/Mo
0.017	5.25E-4
0.033	8.6E-4
0.067	0.00112
0.133	0.00181
0.25	0.00299
0.5	0.00569
1	0.0105
1.5	0.0151
2.5	0.0221
4	0.0303
5.55	0.0379
7.58	0.0444
24.3	0.0796
32.2	0.0913
52.5	0.115
96.4	0.156
193	0.225
362	0.304
607	0.394
866	0.47
1175	0.547
1536	0.627
1922	0.698
2382	0.766
2886	0.829
3623	0.885
4302	0.891

2210600
LPE/BHT/CO/60C/L

t, h	Mt/Mo
0.017	0.00443
0.033	0.00729
0.067	0.0124
0.133	0.0186
0.25	0.0317
0.5	0.0577
1	0.0917
1.5	0.117
2.5	0.158
4	0.202
5.5	0.239
8.03	0.294
24.1	0.513
32	0.604
32	0.604
50.1	0.743
97.7	0.909
218	0.952
386	0.954
606	0.964
1085	0.968

2220300
LPE/BHT/EN/30C/L

t, h	Mt/Mo
0.017	0.00102
0.033	0.00183
0.067	0.00191
0.133	0.00343
0.25	0.00506
0.517	0.00854
1	0.0148
2	0.0226
4	0.0365
6	0.0503
7.5	0.059
23.8	0.103
30	0.113
48.9	0.139
72	0.174
193	0.241
385	0.319
601	0.391
750	0.433
913	0.473
1057	0.513
1228	0.545
1345	0.574
1537	0.604
1708	0.626
1897	0.659
2089	0.683
2405	0.714
2713	0.741
3004	0.768
3360	0.788
4056	0.827
4756	0.848

2220600
LPE/BHT/EN/60C/L

t, h	Mt/Mo
0.017	0.0101
0.033	0.0148
0.067	0.024
0.133	0.0379
0.25	0.0589
0.5	0.089
1	0.125
2	0.174
4	0.239
6	0.292
8	0.346
24	0.56
31.7	0.643
48	0.748
169	0.855
361	0.885
577	0.904
748	0.892
912	0.892
1033	0.926
1204	0.908
1519	0.945

2230300
LPE/BHT/HP/30C/L

t, h	Mt/Mo
0.017	0.0156
0.033	0.0281
0.067	0.045
0.117	0.0687
0.183	0.0984
0.25	0.126
0.333	0.16
0.417	0.196
0.5	0.232
0.667	0.311
0.833	0.402
1	0.506
1.17	0.606
1.33	0.683
1.5	0.748
1.75	0.817
2	0.857
2.25	0.889
2.5	0.908
3.55	0.94
5	0.952
7.5	0.96
12.6	0.96
24	0.959
97.1	0.957

2230301
LPE/BHT/HP/30C/U

t, h	Mt/Mo
0.017	0.0306
0.033	0.0508
0.067	0.0822
0.117	0.119
0.183	0.162
0.25	0.2
0.5	0.335
0.75	0.482
1	0.646
1.5	0.839
2	0.912
2.5	0.94
4	0.958
5.5	0.961
8	0.962
24.3	0.963
32	0.963
48.8	0.963
168	0.964
222	0.964
341	0.964
506	0.965

2230601
LPE/BHT/HP/60C/U

t, h	Mt/Mo
0.017	0.128
0.033	0.19
0.067	0.287
0.133	0.439
0.25	0.704
0.5	0.927
1.03	0.96
2	0.962
3.75	0.962
7	0.963
24	0.963

2250300 LPE/BHT/ON/30C/L		2250600 LPE/BHT/ON/60C/L1		2250602 LPE/BHT/ON/60C/L2	
t, h	Mt/Mo	t, h	Mt/Mo	t, h	Mt/Mo
0.067	0.0011	0.067	0.0282	0.017	0.00322
0.117	0.0017	0.133	0.0391	0.033	0.00507
0.183	0.00276	0.25	0.0569	0.067	0.00722
0.3	0.00405	0.5	0.0859	0.117	0.0109
0.5	0.00699	1	0.131	0.183	0.0161
0.85	0.0115	2	0.203	0.3	0.0254
1.45	0.0167	4	0.322	0.5	0.0434
2.5	0.0264	7	0.473	0.833	0.0716
4.25	0.0388	23.8	0.879	1.5	0.119
6.5	0.0507	28.9	0.898	2.5	0.185
24.6	0.124	47.7	0.923	4	0.275
30.6	0.143	82.4	0.928	5.75	0.372
54.5	0.222	120	0.927	8	0.492
124	0.498	193	0.912	24.1	0.865
216	0.725	289	0.944	32	0.893
384	0.854			56	0.914
624	0.885			120	0.93
865	0.896			217	0.931
1179	0.904			385	0.932
1589	0.918				

2260300
LPE/BHT/TB/30C/L

t, h	Mt/Mo
0.133	0.00181
0.25	0.00216
0.5	0.00356
1	0.00487
2.02	0.00805
4.03	0.0113
5.38	0.0132
6.7	0.0153
24.3	0.0319
30.4	0.0378
51.7	0.0518
72.5	0.0653
169	0.112
316	0.166
410	0.196
576	0.25
724	0.289
889	0.342
1255	0.434
1661	0.531
1901	0.591
2161	0.62
2545	0.675
3169	0.733
3365	0.753

2260600
LPE/BHT/TB/60C/L

t, h	Mt/Mo
0.017	0.00616
0.033	0.00737
0.067	0.0136
0.117	0.0197
0.183	0.0272
0.25	0.035
0.5	0.0618
0.75	0.0797
1	0.094
1.5	0.118
2	0.137
2.5	0.155
3.5	0.185
5.5	0.239
8.33	0.301
24.4	0.529
32.4	0.617
48.8	0.744
80.5	0.867
147	0.923
225	0.931
388	0.937
577	0.931
702	0.942

2280300
LPE/BHT/AQ/30C/L

t, h	Mt/Mo
0.25	0.00167
0.5	0.00281
1	0.00374
2	0.00555
4	0.00788
7.28	0.0116
27.9	0.0175
48.8	0.0223
76.3	0.0268
193	0.0447
364	0.0656
481	0.0729
912	0.106
1225	0.13
1585	0.15
2331	0.185
3028	0.216
3677	0.239
4373	0.251
5113	0.265
5404	0.318

2280600
LPE/BHT/AQ/60C/L

t, h	Mt/Mo
0.25	0.0102
0.5	0.0172
1	0.0229
2	0.0265
4	0.0379
5.75	0.0465
24	0.127
31.4	0.157
52	0.225
121	0.407
172	0.491
216	0.575
337	0.362
508	0.758
625	0.833
1056	0.903
1369	0.906
1729	0.899
2475	0.855
3220	0.878

2310300
BPE/BHT/CO/30C/L

t, h	Mt/Mo
0.017	1.0E-3
0.033	0.00129
0.067	0.00202
0.133	0.00377
0.25	0.00552
0.5	0.00694
1	0.00968
2	0.0148
4	0.0226
6.02	0.0337
7.5	0.0374
24	0.0748
29.5	0.0867
97.1	0.197
145	0.257
193	0.307
364	0.425
533	0.531
821	0.619
1033	0.659
2017	0.697
2017	0.696

2310600
BPE/BHT/CO/60C/L

t, h	Mt/Mo
0.017	0.0125
0.033	0.00857
0.067	0.0134
0.133	0.0219
0.25	0.0283
0.483	0.0557
0.983	0.088
2	0.147
4	0.247
6	0.329
7.5	0.379
24.1	0.677
30.4	0.721
48	0.772
125	0.81
220	0.804
292	0.804
565	0.802
893	0.81
1924	0.776
1924	0.775

2320300
BPE/BHT/EN/30C/L

t, h	Mt/Mo
0.017	0.00187
0.033	0.00255
0.067	0.00355
0.133	0.00526
0.25	0.00685
0.5	0.00943
1.03	0.0137
1.5	0.0171
2.5	0.0226
4	0.0303
6	0.0398
7	0.0438
24	0.0977
48	0.161
54.8	0.178
121	0.302
220	0.434
388	0.581
555	0.667
817	0.733
1037	0.774
1206	0.785
1565	0.796
2065	0.814
2716	0.817
2716	0.822

2320600
BPE/BHT/EN/60C/L1

t, h	Mt/Mo
0.017	0.00779
0.033	0.00937
0.067	0.0166
0.133	0.0232
0.25	0.0343
0.5	0.0584
1	0.0999
1.5	0.137
2.22	0.186
3	0.233
4	0.291
6	0.388
7	0.432
24	0.708
30	0.755
96	0.791
120	0.769
144	0.783
168	0.773
197	0.783
313	0.781
435	0.766
700	0.742
2043	0.755

2320602
BPE/BHT/EN/60C/L2

t, h	Mt/Mo
0.017	0.00603
0.033	0.00763
0.067	0.0111
0.133	0.0169
0.25	0.0265
0.5	0.0437
1	0.0766
1.5	0.106
2.5	0.156
4	0.22
6	0.295
7.75	0.356
25	0.563
30	0.614
120	0.651
318	0.636
532	0.642
1153	0.618
1519	0.614
1972	0.679
1972	0.687

2330301 BPE/BHT/HP/30C/U		2330601 BPE/BHT/HP/60C/U1		2330602 BPE/BHT/HP/60C/U2		2330603 BPE/BHT/HP/60C/U3	
t, h	Mt/Mo	t, h	Mt/Mo	t, h	Mt/Mo	t, h	Mt/Mo
0.017	0.00947	0.017	0.0548	0.017	0.0408	0.017	0.0317
0.033	0.015	0.033	0.0918	0.033	0.0657	0.033	0.0551
0.067	0.0244	0.067	0.153	0.067	0.115	0.067	0.0991
0.117	0.0364	0.117	0.231	0.136	0.2	0.133	0.178
0.183	0.0492	0.183	0.318	0.25	0.337	0.283	0.349
0.25	0.0627	0.25	0.401	0.5	0.604	0.5	0.555
0.5	0.108	0.5	0.661	1	0.751	1	0.675
0.75	0.151	0.783	0.779	2.2	0.769	2.02	0.688
1	0.192	1	0.808	4	0.77	4.25	0.69
1.5	0.273	1.5	0.822	7	0.771	6	0.691
2	0.359	2	0.824	24	0.773	8	0.691
2.5	0.449	2.5	0.825	48.1	0.774	24.5	0.693
4	0.65	4	0.826	124	0.776	32	0.694
5.5	0.741	5.5	0.826	220	0.777	76.8	0.696
8	0.792	8	0.826			366	0.7
24.1	0.812	23.8	0.828			578	0.702
48	0.814	31.9	0.828			991	0.705
80.9	0.814	47.9	0.828			1609	0.708
249	0.815	80.3	0.829			2329	0.711
384	0.816	144	0.83			3025	0.716
557	0.817	225	0.831			3745	0.719
		388	0.832			4515	0.723
		395	0.833			4757	0.724
		702	0.834				

2370300
BPE/BHT/TO/30C/L

t, h	Mt/Mo
0.017	0.00103
0.033	0.0015
0.067	0.00228
0.133	0.00284
0.25	0.00391
0.5	0.00565
1.03	0.00809
1.5	0.0104
2.5	0.0142
4	0.0194
6	0.0249
7.5	0.0294
24	0.0711
31	0.0889
48	0.124
125	0.255
313	0.443
533	0.582
793	0.658
1237	0.704
1561	0.699
2524	0.731
2524	0.731

2370600
BPE/BHT/TO/60C/L

t, h	Mt/Mo
0.017	0.00764
0.033	0.00889
0.067	0.0145
0.133	0.0217
0.25	0.0365
0.5	0.061
1	0.0995
2	0.16
4	0.265
6	0.349
7.5	0.403
23.8	0.67
31	0.701
47.8	0.725
77.4	0.732
151	0.747
244	0.751
412	0.749
484	0.746
757	0.748
1084	0.773
2020	0.76
2020	0.762

2380600
BPE/BHT/AQ/60C/L

t, h	Mt/Mo
1	0.0137
2.07	0.0195
4	0.0263
6.5	0.0346
24.4	0.0602
97.8	0.088
373	0.141
701	0.211
1970	0.378
2000	0.412
2000	0.417
2717	0.508

2430601
BPE/BHT/HP/60C/U1

t, h	Mt/Mo
0.017	0.0238
0.033	0.0412
0.067	0.0755
0.133	0.101
0.25	0.109
0.5	0.112
1.02	0.115
2	0.116
4	0.118
6.08	0.119
8	0.119
24.5	0.121
25.7	0.121

2430602
BPE/BHT/HP/60C/U2

t, h	Mt/Mo
0.017	0.0253
0.033	0.0441
0.067	0.0816
0.133	0.111
0.25	0.118
0.5	0.122
1	0.124
2	0.126
4.25	0.127
6	0.128
7.27	0.128
24.1	0.13
25	0.13

2510300
BPE/BHT/CO/30C/L

t, h	Mt/Mo
0.017	0.00611
0.033	0.00915
0.067	0.0163
0.133	0.0236
0.25	0.0342
0.5	0.0475
1	0.0698
1.5	0.0862
2.5	0.113
3.5	0.139
5.78	0.179
8.5	0.227
24.9	0.41
32.3	0.479
48.4	0.593
80.3	0.74
144	0.887
221	0.964
393	0.998
577	1.01
866	1.01
1207	0.989

2510600
BPE/BHT/CO/60C/L

t, h	Mt/Mo
0.017	0.0361
0.033	0.0501
0.067	0.0722
0.117	0.0956
0.183	0.119
0.25	0.152
0.5	0.253
0.75	0.334
1	0.401
1.5	0.518
2	0.613
2.5	0.691
3.5	0.805
5.5	0.926
8.5	0.987
24.4	0.998
32.6	1
48.5	1.01
56.4	1.01
96.4	1
294	0.993

2520300
BPE/BHT/EN/30C/L

t, h	Mt/Mo
0.017	0.0105
0.033	0.0157
0.067	0.0235
0.117	0.0313
0.183	0.0378
0.25	0.0441
0.5	0.0618
0.75	0.074
1	0.0855
1.5	0.106
2	0.122
2.5	0.139
4	0.177
5.5	0.211
8	0.259
25.8	0.488
38	0.599
55.2	0.709
148	0.931
288	1
384	0.992
649	1
866	0.996
1177	1
1566	0.998
2022	0.99

2520600
BPE/BHT/EN/60C/L1

t, h	Mt/Mo
0.017	0.0534
0.033	0.0675
0.067	0.0914
0.117	0.118
0.183	0.153
0.25	0.183
0.5	0.304
0.75	0.392
1	0.469
1.5	0.597
2	0.702
2.5	0.768
4	0.905
5.5	0.962
8	0.989
24	1.01
32	1.01
55	1.01
120	1
216	1
361	0.999
650	0.994

2520602
BPE/BHT/EN/60C/L2

t, h	Mt/Mo
0.017	0.042
0.033	0.0578
0.067	0.0749
0.117	0.0997
0.183	0.132
0.25	0.159
0.5	0.277
0.75	0.363
1	0.44
1.5	0.57
2	0.669
2.5	0.737
3.5	0.844
5.5	0.945
8.47	0.986
24.4	1.01
32.1	1.01
48.2	1.01
56.5	1
123	1.01
218	1
386	0.993

2595300
BPE/BHT/.95EN/30C/L

t, h	Mt/Mo
0.033	0.00222
0.067	0.00751
0.133	0.0118
0.25	0.021
0.5	0.0286
1	0.0435
2	0.0658
3.97	0.103
5.48	0.13
24.4	0.324
30.1	0.384
53.2	0.523
125	0.744
292	0.877
480	0.919
649	0.915
700	0.93

2595600
BPE/BHT/.95EN/60C/L

t, h	Mt/Mo
0.017	0.032
0.033	0.0438
0.067	0.071
0.133	0.11
0.25	0.161
0.5	0.259
1	0.396
1.95	0.577
4	0.786
5.5	0.85
6.75	0.881
24.3	0.916
30	0.919
96.6	0.912
145	0.934

2530301
BPE/BHT/HP/30C/U

t, h	Mt/Mo
0.017	0.0538
0.033	0.0797
0.067	0.127
0.117	0.192
0.183	0.273
0.25	0.353
0.5	0.683
1	0.942
1.5	0.982
2	0.989
2.5	0.991
4	0.992
5.5	0.993
8.1	0.993
24	0.993
32	0.993
53.9	0.993

2530601
BPE/BHT/HP/60C/U

t, h	Mt/Mo
0.017	0.24
0.033	0.382
0.067	0.616
0.133	0.9
0.25	0.961
0.5	0.964
1	0.965
2	0.965
4	0.965
6	0.965
7.5	0.965
24.3	0.965
52.2	0.965

2550300
BPE/BHT/ON/30C/L

t, h	Mt/Mo
0.017	0.00479
0.033	0.00718
0.067	0.0114
0.117	0.0179
0.183	0.021
0.3	0.029
0.5	0.0394
0.833	0.0579
1.5	0.0868
2.5	0.123
4.27	0.18
7.07	0.25
23.8	0.513
31	0.603
55.1	0.799
120	0.936
216	0.966
385	0.974
554	0.982
865	0.972
1182	0.982

2550600
BPE/BHT/ON/60C/L1

t, h	Mt/Mo
0.017	0.0582
0.033	0.0754
0.067	0.106
0.133	0.151
0.25	0.218
0.5	0.346
1	0.551
1.88	0.771
4	0.944
6	0.964
7.58	0.968
23.9	0.955
29.9	0.982
51.5	1.12
72.3	0.968
145	0.965
216	0.962
385	0.969

2550602
BPE/BHT/ON/60C/L2

t, h	Mt/Mo
0.017	0.0275
0.033	0.041
0.067	0.0566
0.117	0.077
0.183	0.111
0.3	0.175
0.5	0.279
0.833	0.434
1.5	0.675
2.5	0.859
3.57	0.944
5	0.973
7	0.986
22.9	0.996
30.9	1
49.4	0.99
96.2	0.998
216	0.997
220	0.979

2560300
BPE/BHT/TB/30C/L

t, h	Mt/Mo
0.067	0.0225
0.133	0.0332
0.25	0.0432
0.5	0.0599
1	0.0842
2	0.118
4	0.17
6	0.214
7.42	0.24
24	0.435
30.6	0.499
48.2	0.609
121	0.84
216	0.939
265	0.965
360	0.971
481	0.971
793	0.977

2560600
BPE/BHT/TB/60C/L

t, h	Mt/Mo
0.017	0.042
0.033	0.0587
0.067	0.0841
0.133	0.12
0.25	0.175
0.5	0.274
1	0.424
2	0.634
4	0.837
6	0.909
7.33	0.931
24	0.952
48	0.950
97	0.937
192	0.935
313	0.934
605	0.933

2580300
BPE/BHT/AQ/30C/L

t, h	Mt/Mo
0.25	0.0085
0.5	0.0106
1	0.0158
2	0.0202
4	0.0272
23.5	0.043
96.6	0.0728
192	0.107
364	0.161
697	0.272
1442	0.4
2139	0.467
2765	0.473
3460	0.425
3768	0.548

2580600
BPE/BHT/AQ/60C/L

t, h	Mt/Mo
0.083	0.00492
0.167	0.00715
0.25	0.00925
0.5	0.0152
1	0.0183
2	0.0216
4	0.0317
7.42	0.0419
24.6	0.0876
55.3	0.155
72.3	0.199
244	0.464
601	0.62
1347	0.795
2044	0.849
2693	0.867
3365	0.868
3580	0.904

2590400 BPE/BHT/HB/40C/L1		2590402 BPE/BHT/HB/40C/L2		2590600 BPE/BHT/HB/60C/L	
t, h	Mt/Mo	t, h	Mt/Mo	t, h	Mt/Mo
0.017	0.00702	0.017	0.00648	0.017	0.03
0.033	0.0188	0.033	0.0145	0.033	0.0579
0.067	0.0206	0.067	0.021	0.067	0.0774
0.133	0.0274	0.133	0.0333	0.133	0.129
0.267	0.0534	0.25	0.0488	0.25	0.197
0.5	0.0747	0.5	0.0796	0.5	0.296
1	0.118	1	0.121	1	0.462
2.42	0.213	1.92	0.182	1.97	0.659
4	0.289	4	0.293	4	0.857
5.45	0.356	6.05	0.381	5.90	0.93
6.75	0.433	7.42	0.428	24.2	0.974
8.95	0.52	24	0.787	30.4	0.969
11.3	0.579	30.3	0.87	49.8	0.976
32	0.874	49.3	0.925	120	0.984
57.9	0.966	124	0.979	216	0.973
126	0.99	318	1	508	0.958
222	0.985	529	0.979		
297	0.993				
630	0.984				

2610600
LPE/BHT/CO/60C/L

t, h	Mt/Mo
0.017	0.00208
0.033	0.00358
0.067	0.00469
0.133	0.0132
0.25	0.0271
0.5	0.0428
1	0.0779
2	0.131
4	0.202
6	0.256
7.75	0.298
23.7	0.548
31.4	0.658
52	0.809
76	0.913
145	0.958
240	0.966
361	0.945
532	0.969
556	0.954
556	0.957
556	0.957

2620600
LPE/BHT/EN/60C/L

t, h	Mt/Mo
0.017	0.00502
0.033	0.00704
0.067	0.0118
0.133	0.0187
0.25	0.0296
0.5	0.0519
1	0.0857
1.97	0.139
4	0.224
6	0.299
7.5	0.355
24	0.638
31.5	0.763
100	0.905
124	0.917
148	0.93
172	0.929
265	0.925
361	0.909
481	0.924
652	0.905
673	0.955

2630301
LPE/BHT/HP/30C/U

t, h	Mt/Mo
0.017	0.0226
0.033	0.0392
0.067	0.0682
0.117	0.104
0.183	0.148
0.25	0.189
0.5	0.334
0.75	0.495
1	0.639
1.5	0.813
2	0.893
2.5	0.929
4	0.96
5.5	0.965
8	0.968
24.1	0.971
31.8	0.971
48.8	0.972
61.6	0.972
150	0.972

2630601
LPE/BHT/HP/60C/U

t, h	Mt/Mo
0.017	0.0998
0.033	0.166
0.067	0.274
0.133	0.464
0.25	0.759
0.5	0.94
1	0.967
2	0.97
4	0.971
6	0.971
7.7	0.971
24	0.972
25	0.972

2710300
PP/BHT/CO/30C/L

t, h	Mt/Mo
7.5	0.00303
25	0.00838
31.5	0.00845
57.1	0.0155
97.4	0.0219
194	0.0354
366	0.059
605	0.0799
871	0.101
1181	0.122
1538	0.14
1946	0.164
2379	0.184
2907	0.208
3484	0.231
4081	0.243
4731	0.28
5426	0.301

2710600
PP/BHT/CO/60C/L

t, h	Mt/Mo
0.033	0.00566
0.067	0.00918
0.133	0.0304
0.25	0.0223
0.5	0.0409
1	0.0636
2	0.0951
4	0.144
6	0.18
7.52	0.202
23.8	0.368
31.5	0.429
48	0.535
55.5	0.574
72.1	0.652
144	0.814
244	0.844
385	0.833
529	0.867
844	0.864

2720300
PP/BHT/EN/30C/L

t, h	Mt/Mo
1	0.00317
1.5	0.00401
2	0.00356
2.5	0.00481
3.5	0.00808
5	0.0108
6.77	0.0147
8.83	0.0177
25.4	0.0398
34.6	0.0493
50.5	0.0641
84.4	0.0919
121	0.116
223	0.168
386	0.222
625	0.278
869	0.326
1181	0.38
1564	0.437
1899	0.484
2407	0.526
2911	0.563
3411	0.589
4156	0.634
4880	0.671
5595	0.692
6340	0.706

2720600
PP/BHT/EN/60C/L

t, h	Mt/Mo
0.017	0.00534
0.033	0.00558
0.067	0.0122
0.133	0.0191
0.25	0.0341
0.5	0.0566
1	0.101
2	0.159
4	0.256
6	0.33
7.53	0.398
24	0.651
31.5	0.724
48.1	0.809
82.6	0.85
121	0.847
220	0.844
361	0.842
505	0.849
702	0.887

2730301
PP/BHT/HP/30C/U

t, h	Mt/Mo
0.021	0.015
0.033	0.0213
0.067	0.0352
0.117	0.0508
0.183	0.0668
0.25	0.0803
0.35	0.0983
0.5	0.123
0.75	0.161
1	0.202
1.42	0.305
2	0.775
2.75	0.865
3.5	0.872
4.67	0.875
6.67	0.877
8.88	0.878
24	0.879
54.1	0.88

2730601
PP/BHT/HP/60C/U

t, h	Mt/Mo
0.017	0.0778
0.033	0.126
0.067	0.21
0.133	0.467
0.25	0.854
0.5	0.881
1	0.884
1.5	0.884
2	0.885
3.5	0.885
5.5	0.885
7.5	0.886
24.1	0.887
51.9	0.887

2760300
PP/BHT/TB/30C/L

t, h	Mt/Mo
1	7.89E-4
1.5	0.00114
2	0.00394
2.5	0.00306
3.5	0.00479
5.02	0.0061
7.17	0.00950
8.67	0.0109
36.5	0.0326
73	0.0539
125	0.0794
242	0.126
412	0.151
606	0.184
875	0.223
1184	0.267
1516	0.309
1922	0.361
2402	0.407
2839	0.457
3339	0.505
4084	0.587
4808	0.65
5547	0.702
6222	0.752
6992	0.717

2760600
PP/BHT/TB/60C/L

t, h	Mt/Mo
0.033	0.00587
0.067	0.00787
0.133	0.0152
0.25	0.0235
0.5	0.0443
1	0.071
1.95	0.113
4.25	0.187
6	0.232
7.42	0.265
24.8	0.555
31.5	0.648
72.7	0.837
99.7	0.842
121	0.856
172	0.86
289	0.867
580	0.882

2780300
PP/BHT/AQ/30C/L

t, h	Mt/Mo
23.2	0.00434
51.5	0.00819
94.3	0.0145
176	0.0206
293	0.0354
432	0.0449
602	0.0545
862	0.0647
1175	0.076
1542	0.086
1948	0.0947
2352	0.11
2855	0.124
3604	0.136
4274	0.145
4997	0.145
5736	0.158
6411	0.152
7231	0.209

2780600
PP/BHT/AQ/60C/L

t, h	Mt/Mo
0.25	0.00254
0.5	0.00312
1	0.0061
2	0.0117
4.12	0.0177
6.33	0.0243
24	0.05
53.2	0.0878
96.5	0.145
176	0.205
337	0.314
505	0.384
673	0.447
865	0.506
1204	0.554
1537	0.56
1873	0.586
2113	0.596
2449	0.595
2617	0.598
2788	0.583

2810300
PP/C18/CO/30C/L

t, h	Mt/Mo
0.017	0.0024
0.033	0.00301
0.067	0.00457
0.117	0.00585
0.183	0.00761
0.25	0.00904
0.417	0.0116
0.667	0.0156
1	0.02
1.5	0.025
2	0.0294
2.75	0.0356
4.05	0.0451
5.5	0.0535
7.67	0.0653
27.4	0.131
34.9	0.151
75	0.228
146	0.309
240	0.388
409	0.491
601	0.569
847	0.646
1179	0.721
1514	0.779
1925	0.834
2402	0.878
3077	0.924
3737	0.951
4471	0.976
5163	0.986
5885	0.996
6625	0.992

2810600
PP/C18/CO/60C/L

t, h	Mt/Mo
0.017	0.0172
0.033	0.0246
0.067	0.0425
0.133	0.048
0.25	0.0945
0.5	0.142
1	0.213
2	0.317
4	0.455
6	0.56
7.5	0.621
24.3	0.886
31.5	0.949
48.8	0.992
145	1
361	0.999

2820300
PP/C18/EN/30C/L

t, h	Mt/Mo
0.017	0.00383
0.033	0.00551
0.067	0.00774
0.117	0.0109
0.183	0.0134
0.25	0.0166
0.417	0.0242
0.667	0.0332
1	0.0425
1.5	0.0542
2	0.0641
2.5	0.0737
4	0.0966
5.77	0.118
7.68	0.14
25.9	0.272
32	0.304
79.2	0.486
127	0.61
243	0.794
408	0.908
602	0.964
873	0.988
1184	1
1517	1
1926	1.01
1999	0.993

2820600
PP/C18/EN/60C/L

t, h	Mt/Mo
0.017	0.017
0.033	0.03
0.067	0.0476
0.133	0.0781
0.25	0.123
0.5	0.195
1	0.308
2	0.48
4	0.7
6.25	0.833
23.4	0.949
31	0.977
51.9	0.957
121	0.955
193	0.936
289	0.941
385	0.996

2830301
PP/C18/HP/30C/U

t, h	Mt/Mo
0.017	0.0378
0.033	0.0573
0.067	0.0853
0.117	0.116
0.183	0.15
0.25	0.18
0.35	0.223
0.5	0.287
0.75	0.426
1	0.908
1.25	0.995
1.5	0.999
1.75	0.999
2	1
2.25	1
2.5	1
2.75	1
3	1
3.5	1
3.98	1
5	1
6.67	1
8.83	1
24	1
31.8	1

2830601
PP/C18/HP/60C/U

t, h	Mt/Mo
0.017	0.128
0.033	0.184
0.067	0.304
0.133	0.708
0.25	0.997
0.5	1
1	1
2	1
22.8	1
51.8	1

2860300
PP/C18/TB/30C/L

t, h	Mt/Mo
0.017	0.00207
0.033	0.00385
0.067	0.00607
0.117	0.00808
0.183	0.0104
0.25	0.0127
0.417	0.0172
0.667	0.0224
1	0.0288
1.5	0.0356
2	0.0408
2.5	0.0464
3.67	0.0578
5.27	0.0699
7.33	0.085
24.1	0.158
31.2	0.181
47.4	0.228
55.2	0.246
144	0.381
218	0.461
388	0.599
608	0.725
868	0.826
1180	0.905
1516	0.954
1902	0.982
2406	0.99
2905	0.99
3409	0.993
4681	0.996

2860600
PP/C18/TB/60C/L

t, h	Mt/Mo
0.017	0.0206
0.033	0.029
0.067	0.0445
0.133	0.064
0.25	0.0958
0.5	0.155
1	0.223
2	0.332
4	0.486
5.98	0.597
7.33	0.668
22.5	0.969
31.4	0.984
48.3	1
72.6	0.995
145	0.973
221	0.998

2880300
PP/C18/AQ/30C/L

t, h	Mt/Mo
TO	
9173	0.0005±0.0002

2880600
PP/C18/AQ/60C/L

t, h	Mt/Mo
27.8	6.7E-4
96.6	7.53E-4
169	6.26E-4
361	8.89E-4
700	9.63E-4
1369	0.00103
2092	0.0011
2113	0.00115
2833	8.92E-4
3941	7.65E-4
4632	8.76E-4
5405	9.7E-4
6072	8.41E-4
6865	8.65E-4
7657	8.42E-4
8760	9.41E-4
9582	9.72E-4

2910300
PP/C32/CO/30C/L

t, h	Mt/Mo
0.017	0.0394
0.033	0.0419
0.067	0.0487
0.117	0.049
0.183	0.0499
0.25	0.0496
0.5	0.0496
1	0.0508
2	0.0519
4	0.0535
7	0.0553
25.3	0.0665
31.3	0.0697
52.6	0.0768
96.7	0.102
201	0.129
337	0.156
577	0.196
840	0.231
1157	0.264
1513	0.3
1922	0.339
2355	0.372
2790	0.408
3462	0.453
4057	0.491
4710	0.538
5401	0.579
6144	0.627
6918	0.672
7374	0.691

2910600
PP/C32/CO/60C/L

t, h	Mt/Mo
0.017	0.0374
0.033	0.0406
0.067	0.0434
0.117	0.0456
0.183	0.0502
0.25	0.0556
0.417	0.0714
0.667	0.0926
1	0.115
1.42	0.14
1.92	0.166
2.53	0.193
3.53	0.234
5	0.282
7.27	0.342
25.7	0.637
52.1	0.867
82.8	0.968
125	0.99
245	0.994
366	0.995

2920300
PP/C32/EN/30C/L

t, h	Mt/Mo
0.017	0.0136
0.033	0.0243
0.067	0.0341
0.133	0.0356
0.25	0.0362
0.5	0.0382
1	0.039
2	0.0441
4	0.0497
6	0.0552
7.5	0.0604
23.8	0.0921
32.6	0.11
53.5	0.138
121	0.201
169	0.239
216	0.279
289	0.313
360	0.36
481	0.412
529	0.441
625	0.481
769	0.533
961	0.587
1108	0.625
1249	0.653
1440	0.687
1633	0.722
1777	0.74
1945	0.751
2113	0.768
2281	0.804
2476	0.769
2644	0.854

2920600
PP/C32/EN/60C/L

t, h	Mt/Mo
0.017	0.0326
0.033	0.0371
0.067	0.0421
0.117	0.0483
0.183	0.059
0.25	0.069
0.417	0.0929
0.667	0.132
1	0.172
1.42	0.219
1.92	0.27
2.75	0.349
3.75	0.434
5.27	0.539
7.25	0.646
23.9	0.942
31.2	0.965
55	0.942
121	0.97
223	0.967
386	0.972
601	0.968
678	0.981

2930301
PP/C32/HP/30C/U

t, h	Mt/Mo
0.017	0.0354
0.033	0.0415
0.067	0.0507
0.15	0.0708
0.25	0.0902
0.5	0.131
1	0.216
1.97	0.813
4	0.986
5.5	0.989
8.67	0.991
24.1	0.993
31.6	0.993
96.5	0.995
121	0.995

2930601
PP/C32/HP/60C/U

t, h	Mt/Mo
0.008	0.0673
0.017	0.0906
0.033	0.132
0.067	0.207
0.1	0.282
0.133	0.401
0.167	0.644
0.2	0.814
0.233	0.906
0.267	0.953
0.3	0.975
0.333	0.986
0.5	0.996
0.833	0.997
1.33	0.997
2	0.997
2.83	0.998
3.9	0.998
19.1	0.998
27.9	0.998
51.9	0.998
73.2	0.998
93.7	0.998

2960300
PP/C32/TB/30C/L

t, h	Mt/Mo
0.017	0.0255
0.033	0.0388
0.067	0.0521
0.117	0.0534
0.183	0.0551
0.3	0.0543
0.5	0.0545
1	0.0553
2	0.0575
4	0.0592
7	0.0636
24.4	0.0701
31	0.0837
52.8	0.101
80.5	0.117
121	0.138
217	0.182
390	0.246
628	0.307
865	0.358
1178	0.426
1540	0.504
2071	0.614
2402	0.674
2931	0.753
3507	0.826
4085	0.879
4730	0.929
5426	0.945
6196	0.957
6964	0.958
7374	0.957

2960600
PP/C32/TB/60C/L

t, h	Mt/Mo
0.017	0.0404
0.033	0.0415
0.067	0.0436
0.117	0.0475
0.2	0.0569
0.333	0.069
0.533	0.0904
0.833	0.116
1.33	0.155
2.08	0.202
3.25	0.261
4.75	0.325
7.25	0.419
24	0.843
31	0.92
58.9	0.977
100	0.983
221	0.988
413	0.991

2980600
PP/C32/AQ/60C/L

t, h	Mt/Mo
TO	
8065	0.0005±0.0002

2980300
PP/C32/AQ/30C/L

t, h	Mt/Mo
4705	5.05E-4
5401	9.73E-4
6125	0.00291
6937	0.00507
8068	0.0085
	0.0164

3040301
PP/C18/OD/30C/U

t, h	Mt/Mo
0.005	0.0294
0.011	0.0639
0.017	0.0785
0.025	0.0975
0.033	0.114
0.05	0.136
0.067	0.157
0.1	0.188
0.133	0.215
0.167	0.238
0.25	0.289
0.333	0.332
0.5	0.406
0.75	0.499
1.02	0.584
1.5	0.701
2	0.786
3	0.89
4.5	0.959
6.25	0.987
8.93	0.997
26.1	1
30.9	1

3040601
PP/C18/OD/60C/U

t, h	Mt/Mo
0.005	0.639
0.011	0.661
0.017	0.672
0.025	0.684
0.033	0.696
0.05	0.714
0.067	0.73
0.1	0.759
0.133	0.785
0.167	0.808
0.25	0.856
0.333	0.891
0.5	0.938
0.75	0.972
1	0.988
1.5	0.998
2	1
3	1
5	1
8.78	1
30.9	1

3110300
E.05VA/BHT/CO/30C/L

t, h	Mt/Mo
0.017	0.00458
0.033	0.0478
0.067	0.0208
0.133	0.0253
0.25	0.0342
0.5	0.0913
1	0.128
1.92	0.207
3.95	0.305
5.85	0.369
7.5	0.426
23.6	0.713
30.7	0.778
48.3	0.839
54.8	0.848
77.5	0.868
144	0.883
222	0.881
341	0.882
384	0.88

3110600
E.05VA/BHT/CO/60C/L

t, h	Mt/Mo
0.017	0.0668
0.033	0.103
0.067	0.155
0.133	0.234
0.25	0.292
0.5	0.478
1.03	0.688
1.98	0.824
3.98	0.865
5.5	0.878
6.83	0.873
24.1	0.867
121	0.877

3120300
E.05VA/BHT/EN/30C/L

t, h	Mt/Mo
0.017	0.0209
0.033	0.03
0.067	0.0413
0.133	0.0629
0.25	0.0871
0.5	0.127
1.02	0.186
1.97	0.263
4	0.392
5.42	0.471
24.1	0.8
30.8	0.845
96.3	0.877
151	0.888
264	0.892
461	0.89
484	0.893

3120600
E.05VA/BHT/EN/60C/L

t, h	Mt/Mo
0.017	0.0824
0.033	0.129
0.067	0.182
0.133	0.262
0.25	0.382
0.5	0.568
1	0.723
1.98	0.864
3.98	0.89
5.52	0.899
6.78	0.894
24.6	0.888
30.5	0.892
49.3	0.878
75.8	0.874
144	0.87
172	0.893

3195600
E.05VA/BHT/.95EN/60C/L

t, h	Mt/Mo
0.017	0.0906
0.033	0.127
0.067	0.173
0.117	0.223
0.183	0.284
0.283	0.369
0.433	0.48
0.667	0.618
1	0.741
1.5	0.84
2	0.88
2.85	0.905
4.25	0.923
6.52	0.921
9.2	0.921
22.5	0.919
32.4	0.922
51.8	0.913

3195300
E.05VA/BHT/.95EN/30C/L

t, h	Mt/Mo
0.017	0.0291
0.033	0.0391
0.067	0.0521
0.117	0.0688
0.183	0.0845
0.283	0.104
0.433	0.127
0.667	0.155
1	0.19
1.5	0.235
2	0.269
3	0.33
4.25	0.394
6	0.473
8.82	0.573
22.5	0.798
32.5	0.853
48.2	0.889
83.3	0.911
145	0.916
217	0.925
384	0.918
581	0.909

3130300
E.05VA/BHT/HP/30C/L

t, h	Mt/Mo
0.017	0.115
0.033	0.171
0.067	0.272
0.133	0.475
0.25	0.758
0.5	0.883
1	0.905
2.05	0.904
3	0.907
4.93	0.902
6.33	0.913
23.2	0.893
30.2	0.893
48.1	0.892
120	0.891
169	0.894

3130301
E.05VA/BHT/HP/30C/U

t, h	Mt/Mo
0.006	0.0472
0.011	0.0721
0.017	0.0938
0.025	0.121
0.033	0.145
0.05	0.187
0.067	0.224
0.1	0.292
0.15	0.386
0.2	0.479
0.3	0.646
0.45	0.786
0.667	0.853
1	0.875
1.5	0.88
2.25	0.882
3.33	0.883
5	0.884
6.5	0.884
8.67	0.884
22.9	0.885
56.2	0.886
128	0.886

3130600
E.05VA/BHT/HP/60C/L

t, h	Mt/Mo
0.008	0.251
0.017	0.358
0.025	0.489
0.033	0.548
0.05	0.678
0.067	0.774
0.083	0.83
0.125	0.882
0.167	0.911
0.25	0.921
0.5	0.896
1	0.895
2.92	0.883
5	0.871
6.67	0.894
24.3	0.831
30.5	0.889
96.2	0.841
121	0.888

3180300
E.05VA/BHT/AQ/30C/L

t, h	Mt/Mo
0.033	0.00503
0.083	0.0074
0.167	0.00891
0.333	0.0122
0.583	0.0142
1.47	0.0219
3.67	0.036
6.62	0.0515
24.4	0.0915
54	0.122
149	0.151
213	0.16
556	0.183
817	0.2
1033	0.22
1321	0.226
1657	0.236
2164	0.257
2763	0.286
3409	0.307
3845	0.343

3180600
E.05VA/BHT/AQ/60C/L

t, h	Mt/Mo
0.033	0.0152
0.083	0.0212
0.167	0.0274
0.25	0.0337
1	0.05
3	0.0792
5.07	0.092
7.12	0.102
24.2	0.122
30.9	0.132
53.5	0.151
120	0.204
198	0.257
293	0.319
457	0.384
700	0.49
961	0.565
1177	0.61
1465	0.656
1801	0.67
2308	0.665
2907	0.688
3479	0.696
3966	0.708

3210300
E.13VA/BHT/CO/30C/L

t, h	Mt/Mo
0.017	0.00949
0.033	0.0123
0.067	0.0209
0.117	0.0297
0.183	0.0364
0.3	0.049
0.5	0.0652
0.833	0.0881
1.33	0.112
2	0.14
3	0.178
4.5	0.221
6.25	0.263
8.5	0.31
23.8	0.532
32.4	0.627
49.6	0.756
82	0.9
121	0.96
223	0.989
390	0.997
651	1
870	1
1183	0.987

3210600
E.13VA/BHT/CO/60C/L

t, h	Mt/Mo
0.017	0.0355
0.033	0.053
0.067	0.0761
0.117	0.107
0.183	0.136
0.283	0.18
0.433	0.237
0.667	0.319
1	0.413
1.5	0.527
2	0.627
3	0.766
4.25	0.876
6	0.954
8.25	1
25.3	1.03
31.9	1.03
54.7	1.03
78.7	0.99

3220300
E.13VA/BHT/EN/30C/L

t, h	Mt/Mo
0.017	0.0178
0.033	0.0257
0.067	0.0362
0.117	0.0492
0.183	0.062
0.3	0.0806
0.5	0.106
0.833	0.138
1.5	0.191
2.5	0.246
4	0.318
5.75	0.389
8	0.468
24.3	0.802
31.9	0.877
48.2	0.975
79.5	0.992
104	0.998
219	1
388	0.999
605	0.989

3220600
E.13VA/BHT/EN/60C/L

t, h	Mt/Mo
0.017	0.0384
0.033	0.0562
0.067	0.0795
0.117	0.12
0.183	0.16
0.25	0.188
0.417	0.282
0.667	0.403
1	0.525
1.52	0.682
2	0.785
2.5	0.856
3.75	0.945
5.5	0.988
7.75	0.999
24.9	0.998
31.6	1
50.7	0.996
96.8	1
198	0.998
365	0.999
461	0.996
535	0.996
703	0.987

3295300
E.13VA/BHT/.95EN/30C/L

t, h	Mt/Mo
0.017	0.0168
0.033	0.0244
0.067	0.0342
0.117	0.0462
0.183	0.0586
0.283	0.0734
0.433	0.0926
0.667	0.115
1	0.142
1.5	0.177
2	0.206
3	0.252
4.25	0.303
6	0.36
8.5	0.432
24.1	0.721
32.6	0.808
47.5	0.9
59.3	0.94
121	0.994
215	0.998
384	0.991
626	0.993
871	0.982

3295600
E.13VA/BHT/.95EN/60C/L

t, h	Mt/Mo
0.017	0.0528
0.033	0.0745
0.067	0.104
0.117	0.137
0.183	0.177
0.283	0.231
0.433	0.303
0.667	0.398
1	0.512
1.5	0.649
2.25	0.788
3.5	0.906
4.75	0.957
6.5	0.978
10.2	0.992
22.5	0.993
34	0.99
49	0.975
53.8	0.98

3230301
E.13VA/BHT/HP/30C/U

t, h	Mt/Mo
0.005	0.0489
0.011	0.0729
0.017	0.0905
0.025	0.113
0.033	0.131
0.05	0.163
0.067	0.191
0.1	0.237
0.15	0.299
0.2	0.353
0.3	0.45
0.45	0.584
0.667	0.758
1	0.904
1.5	0.969
2.25	0.984
3.5	0.986
4.8	0.986
7	0.987
22	0.987
31	0.987
53.2	0.987
98.1	0.987
196	0.987

3230601
E.13VA/BHT/HP/60C/U

t, h	Mt/Mo
0.005	0.126
0.011	0.191
0.017	0.243
0.025	0.308
0.033	0.365
0.05	0.463
0.067	0.55
0.1	0.703
0.133	0.816
0.167	0.886
0.2	0.932
0.233	0.956
0.283	0.975
0.35	0.983
0.433	0.986
0.55	0.987
0.683	0.988
0.85	0.988
1.05	0.988
1.3	0.988
1.6	0.988
2	0.988
3	0.989
4.05	0.989
6	0.989
9	0.989

3280300
E.13VA/BHT/AQ/30C/L

t, h	Mt/Mo
0.033	1.83E-4
0.083	3.95E-4
0.167	6.09E-4
0.333	8.37E-4
0.667	0.00162
1.33	0.00213
2.57	0.00316
4.5	0.0044
7.75	0.00571
23.5	0.00739
31.3	0.0101
55.7	0.0114
121	0.0142
216	0.0165
389	0.0199
627	0.0229
865	0.0263
1183	0.0305
1536	0.036
1968	0.0398
2401	0.0432
2907	0.0496
3462	0.0618

3280600
E.13VA/BHT/AQ/60C/L

t, h	Mt/Mo
0.083	5.78E-4
0.167	0.00148
0.333	0.00172
0.667	0.00284
1	0.00373
1.5	0.00456
2.25	0.00611
3.75	0.00764
5.33	0.00874
7.25	0.00952
22.5	0.0129
31.1	0.0137
46.5	0.0152
98.2	0.0199
223	0.0342
385	0.0491
582	0.0664
871	0.0998
1176	0.131
1536	0.176
1919	0.216
2408	0.265
2904	0.313
3415	0.371

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11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

Food packaging is an inseparable part of modern life. Any substance that migrates from the packaging material into foods is viewed as indirect food additives. In connection with toxicological knowledge, it is important to know the amount of such indirect food additives expected to be present in the food during storage and processing. This program, sponsored by the Bureau of Foods of the Food and Drug Administration is to provide theoretical models, reliable data base, methodology to study the migration phenomena and to provide reasonable worst-case estimates for the concentrations of the indirect additives in food. In this final report we present the results of approximately 250 completed migration experiments based on radiotracer techniques on the migration of low molecular weight hydrocarbons and antioxidants from polyethylene, polypropylene and ethylene-vinyl acetate copolymers. Results of a study for the determination of relative diffusion coefficients of several probe molecules in the polyethylene melt by inverse gas chromatography are also presented. Based on these studies, ethanol appears to be a far more reasonable food-oil stimulating solvent than n-heptane. Other pure or mixed triglycerides may also be considered as food-oil simulating solvents, however they may pose the same analytical difficulties as that of the food oil itself.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

antioxidants; diffusion; ethylene-vinyl acetate copolymers; food packaging; inverse gas chromatography; migration; oligomers; polyethylene; polypropylene; radiotracer

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